Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: K Sanders Examiner # : 60941 Date: 7/7/03
Art Unit: 1714 Phone Number 308-2435 Serial Number: 09/184,464
Mail Box and Bldg/Room Location: CP3 4D17 Results Format Preferred (circle): PAPER DISK E-MAIL

If mor than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Benzo-furan-2-one.

Inventors (please provide full names): _____

Earliest Priority Filing Date: 3/03/00

***For Sequence Searches Only** Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Follow-up search to earlier search.

STAFF USE ONLY

Searcher: Claire
Searcher Phone #: _____
Searcher Location: _____
Date Searcher Picked Up: 7/10/03
Date Completed: 7/10/03
Searcher Prep & Review Time: 120 mn
Clerical Prep Time: _____
Online Time: 120 mn

Type of Search

NA Sequence (#) _____
AA Sequence (#) ✓
Structure (#) _____
Bibliographic _____
Litigation _____
Fulltext _____
Patent Family _____
Other _____

Vendors and cost where applicable

STN ✓
Dialog _____
Questel/Orbit _____
Dr.Link _____
Lexis/Nexis _____
Sequence Systems _____
WWW/Internet _____
Other (specify) _____

PTO-1590 (8-01)

STIC Search Report
EIC 1700

USPTO

STIC Database Tracking Number: 98260

TO: Kriellion Sanders
Location:
Art Unit: 1714
July 10, 2003

Case Serial Number: 09/518464

From: John Calve
Location: EIC 1700
CP3/4-3D62
Phone: 703-308-4139

John.calve@uspto.gov

Search Notes

Hello,

This search is a more general structure search. The search yielded 566 registry numbers, which were "crossed over" into HCA (Chemical Abstracts). I got 265 records (journals, patents…) in HCA that had at least one of the 566 registry numbers indexed or referenced. Since the number of records was too high to print I tried to reduce this number as much as possible. The records were printed out in the following order:

1. First I printed out the authors record, so you could see the compounds. (L26)
2. A few records of a compound that was referenced in many documents. (L41). This was done to reduce the final answer set (L49).
3. A few records for compounds that weren't close enough to the authors compounds. (L47)
4. The main set of answers L49, since there were 169 answers I printed a sample of these answers.

↳ begin on pg 25 of the handout

I believe the printout contains compounds that you can use to reject claim 1.

I also took the registry numbers from the author's record (the species classified or indexed by CA) and Searched them in HCA. To my surprise, I found only the authors record.

If you have any concerns please call me at your convenience. Thanks.

John

sira
Search and Information Resources Administration

STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact ***the EIC searcher or contact:***

Kathleen Fuller, EIC 1700 Team Leader
308-4290, CP3/4-3D62

Structure Search

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1713*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

- *Relevant prior art **not found:***
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to STIC/EIC1700 CP3/4 3D62

```
=> file reg

FILE 'REGISTRY' ENTERED AT 15:04:29 ON 08 JUL 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     7 JUL 2003  HIGHEST RN 544408-69-7
DICTIONARY FILE UPDATES:    7 JUL 2003  HIGHEST RN 544408-69-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.



=> d his

     (FILE 'HOME' ENTERED AT 13:36:54 ON 10 JUL 2003)

     FILE 'LREGISTRY' ENTERED AT 13:36:58 ON 10 JUL 2003
L1              STR

     FILE 'REGISTRY' ENTERED AT 13:40:36 ON 10 JUL 2003
L2            8 S L1

************************************************************
L3 is the structure search - in registry file. L4 is the number of
records in Chemical abstracts that indexed or referenced these reg.
numbers.
************************************************************

L3          566 S L1 FULL
                SAVE L3 SANDERS464/A

     FILE 'HCA' ENTERED AT 13:42:14 ON 10 JUL 2003
L4          265 S L3
L5           46 S L4 AND P/DT
L6          219 S L4 NOT L5
L7          199 S L6 AND 1907-1999/PY
L8           25 S L5 AND 1907-1999/PY
L9          224 S FEILER ?/AU
L10         742 S RUCH ?/AU
L11          70 S WALLQUIST ?/AU
L12         228 S NESVADBA ?/AU
L13           1 S L9 AND L10 AND L11 AND L12
                SEL L13 RN

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L14         106 S E1-E106
L15          60 S L14 AND 3-10/NR
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L17           21 S L16 NOT L3
L18           39 S L15 NOT L17

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L20         1381 S L15

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L21       108179 S 333.200?/RID
L22           44 S L15 AND L21
L23            5 S L22 NOT L18

     FILE 'HCA' ENTERED AT 13:48:51 ON 10 JUL 2003
L24            1 S L23
L25            1 S L19 OR L24
L26            1 S L13 AND L3
L27          224 S L4 AND 1907-1999/PY
L28          ANALYZE L27 1-224 RN :    4681 TERMS


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L29            1 S E3
                E 553-86-6/RN
L30            1 S E3
                E 6273-79-6/RN
L31            1 S E3
                E 521-52-8/RN
L32            1 S E3
L33            3 S (L30 OR L31 OR L32)
L34            1 S L33 AND L21
L35          566 S L3 AND L21
                E 26548-70-9/RN
L36            1 S E3
L37          565 S L3 NOT 10091-92-6/RN

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L38          233 S L37
L39           32 S L4 NOT L38
L40          194 S L38 AND 1907-1999/PY
L41           30 S L39 AND 1907-1999/PY


     FILE 'REGISTRY' ENTERED AT 14:03:22 ON 10 JUL 2003
L42          565 S L37 NOT (26548-70-9 OR 125-46-2 OR 18463-11-1 OR 479-20-9 OR
L43          565 S L37 NOT (1099-45-2 OR 614-75-5 OR 84-24-2)
L44           33 S L43 AND 0-10/C
L45          532 S L43 NOT L44

     FILE 'HCA' ENTERED AT 14:17:58 ON 10 JUL 2003
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L47           41 S L46 AND 1907-1999/PY
L48          196 S L45
L49          169 S L48 AND 1907-1999/PY

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=> d que stat L3
L1              STR
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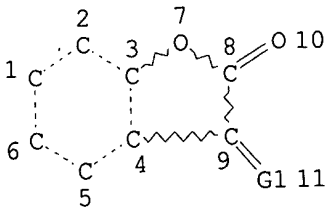


C @13 N @15 Hy @17

VAR G1=13/15/17
NODE ATTRIBUTES:
NSPEC IS RC AT 13
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 9
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L3 566 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 74109 ITERATIONS 566 ANSWERS
SEARCH TIME: 00.00.02

=> file hca
FILE 'HCA' ENTERED AT 14:19:57 ON 10 JUL 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 3 Jul 2003 VOL 139 ISS 2
FILE LAST UPDATED: 3 Jul 2003 (20030703/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

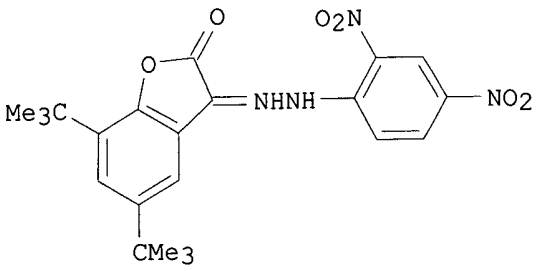
=> d L26 cbib abs hitstr

(Authors Record)

L26 ANSWER 1 OF 1 HCA COPYRIGHT 2003 ACS
133:239371 2-Benzofuranones as styryl dye analogs, their preparation and use.
Feiler, Leonhard; Ruch, Thomas; Wallquist, Olof ; Nesvadba, Peter (Ciba Specialty Chemicals Holding Inc., Switz.). PCT Int. Appl. WO 2000053597 A2 20000914, 102 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,

IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-EP1808 20000302. PRIORITY: CH 1999-447 19990310.

GI



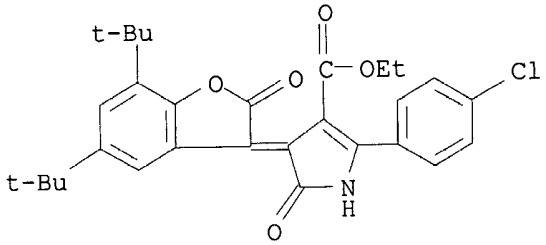
II

AB Polymethine or azomethine dyes contg. 2-oxobenzofuran-3-ylidene moieties, in which the arom. ring of the benzofuran system may be substituted with monovalent substituents or with fused rings, are useful as dyes in inks, mineral oils, plastics, etc. Thus, 2,4-di-tert-butylphenol was cyclocondensed with glyoxylic acid to produce 5,7-di-tert-butyl-3-hydroxy-2-benzofuranone, which was oxidized to 5,7-di-tert-butyl-2,3-benzofurandione (I). Condensation of I with 2,4-(O2N)2C6H3NHNH2 gave yellow II, .lambda.max 434 nm. Many related dyes were similarly prepd.

IT **293750-61-5P**
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(claret; prepn. of benzofuranone derivs. as styryl dye analogs)

RN 293750-61-5 HCA

CN 1H-Pyrrole-3-carboxylic acid, 4-[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]-2-(4-chlorophenyl)-4,5-dihydro-5-oxo-, ethyl ester (9CI) (CA INDEX NAME)

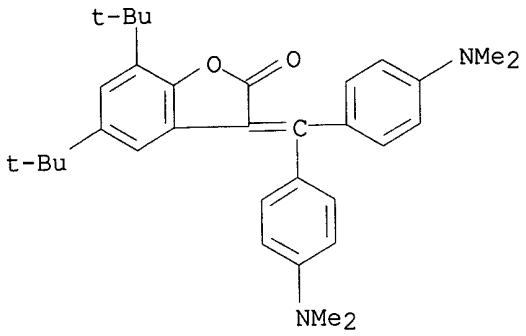


IT **293750-22-8P 293750-23-9P 293750-30-8P**
293750-32-0P 293750-36-4P 293750-42-2P
293750-57-9P 293750-64-8P 293750-65-9P
293750-68-2P 293750-70-6P 293750-73-9P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(orange; prepn. of benzofuranone derivs. as styryl dye analogs)

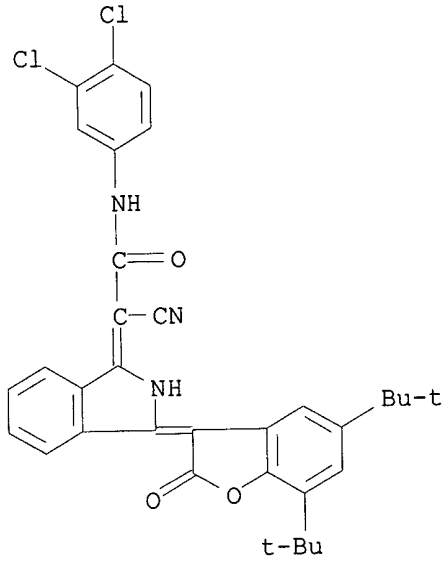
RN 293750-22-8 HCA

CN 2(3H)-Benzofuranone, 3-[bis[4-(dimethylamino)phenyl]methylene]-5,7-bis(1,1-

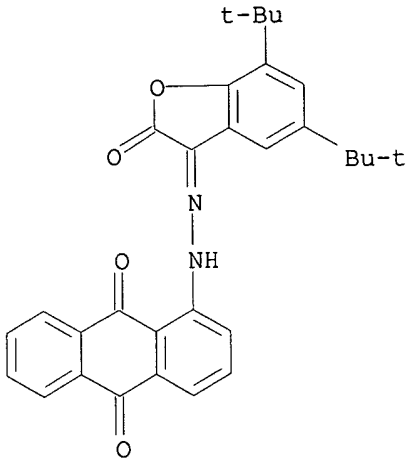
dimethylethyl)- (9CI) (CA INDEX NAME)



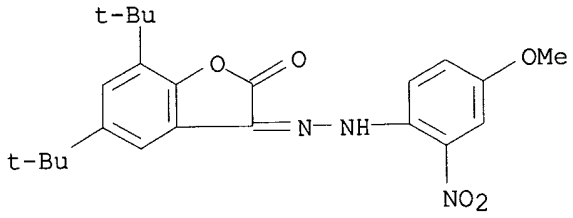
RN 293750-23-9 HCA
CN Acetamide, 2-[3-[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]-2,3-dihydro-1H-isoindol-1-ylidene]-2-cyano-N-(3,4-dichlorophenyl)- (9CI) (CA INDEX NAME)



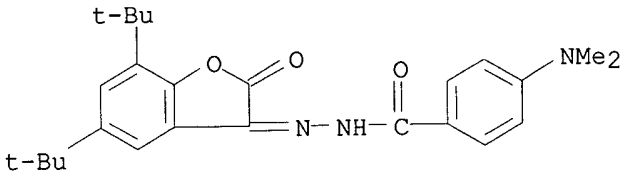
RN 293750-30-8 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[(9,10-dihydro-9,10-dioxo-1-anthracenyl)hydrazone] (9CI) (CA INDEX NAME)



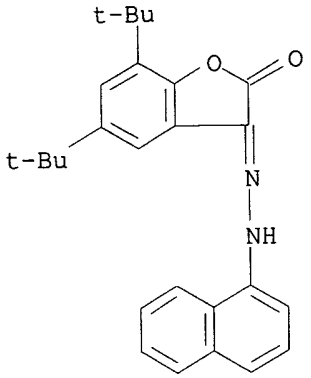
RN 293750-32-0 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[(4-methoxy-2-nitrophenyl)hydrazone] (9CI) (CA INDEX NAME)



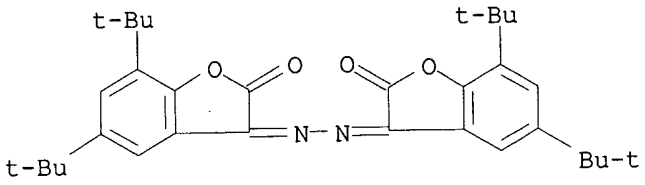
RN 293750-36-4 HCA
CN Benzoic acid, 4-(dimethylamino)-, [5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]hydrazide (9CI) (CA INDEX NAME)



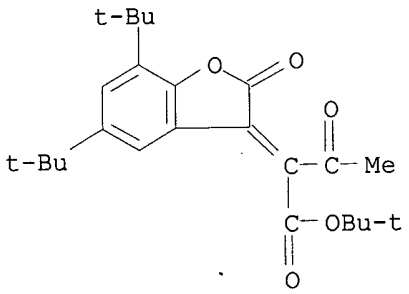
RN 293750-42-2 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-(1-naphthalenylhydrazone) (9CI) (CA INDEX NAME)



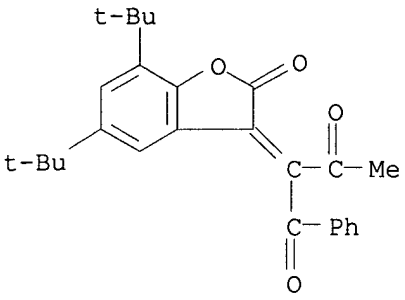
RN 293750-57-9 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]hydrazone] (9CI) (CA INDEX NAME)



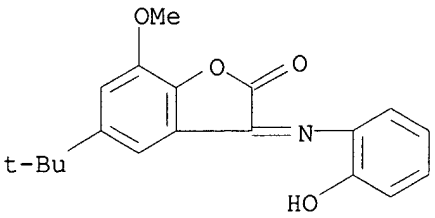
RN 293750-64-8 HCA
CN Butanoic acid, 2-[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]-3-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



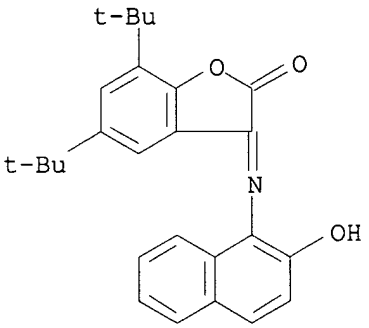
RN 293750-65-9 HCA
CN 1,3-Butanedione, 2-[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]-1-phenyl- (9CI) (CA INDEX NAME)



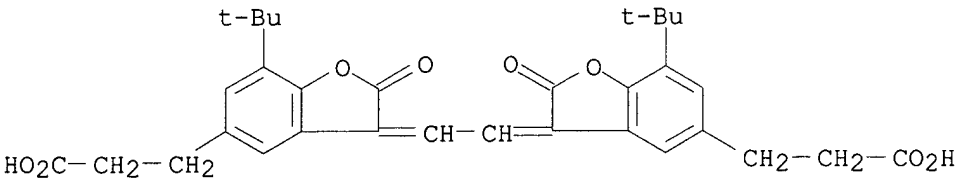
RN 293750-68-2 HCA
CN 2(3H)-Benzofuranone, 5-(1,1-dimethylethyl)-3-[(2-hydroxyphenyl)imino]-7-methoxy- (9CI) (CA INDEX NAME)



RN 293750-70-6 HCA
CN 2(3H)-Benzofuranone, 5,7-bis(1,1-dimethylethyl)-3-[(2-hydroxy-1-naphthalenyl)imino]- (9CI) (CA INDEX NAME)



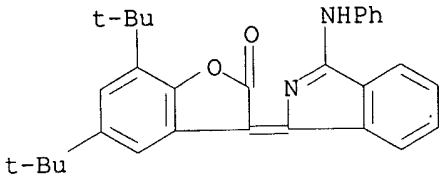
RN 293750-73-9 HCA
CN 5-Benzofuranpropanoic acid, 3,3'-(1,2-ethanediylidene)bis[7-(1,1-dimethylethyl)-2,3-dihydro-2-oxo- (9CI) (CA INDEX NAME)



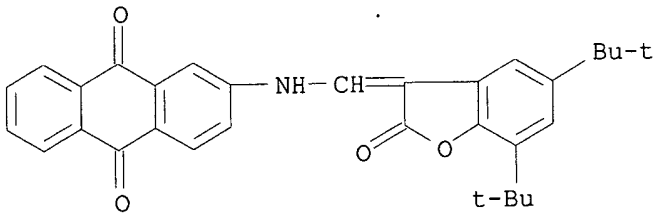
IT **293750-25-1P 293750-26-2P 293750-27-3P 293750-58-0P 293750-69-3P 293750-71-7P 293750-72-8P**

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(red; prepn. of benzofuranone derivs. as styryl dye analogs)

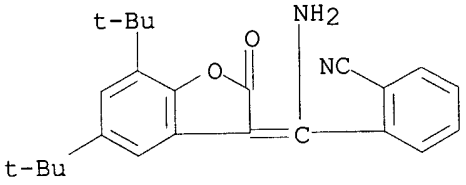
RN 293750-25-1 HCA
CN 2(3H)-Benzofuranone, 5,7-bis(1,1-dimethylethyl)-3-[3-(phenylamino)-1H-isoindol-1-ylidene]- (9CI) (CA INDEX NAME)



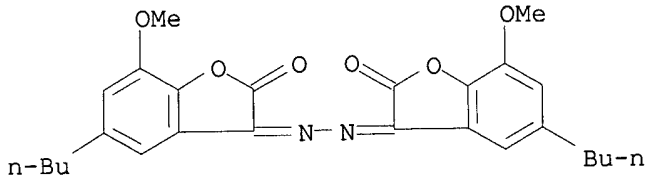
RN 293750-26-2 HCA
CN 9,10-Anthracenedione, 2-[[[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]methyl]amino]- (9CI) (CA INDEX NAME)



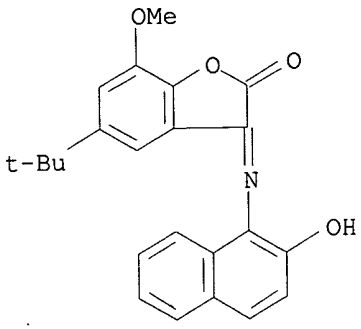
RN 293750-27-3 HCA
CN Benzonitrile, 2-[amino[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]methyl]- (9CI) (CA INDEX NAME)



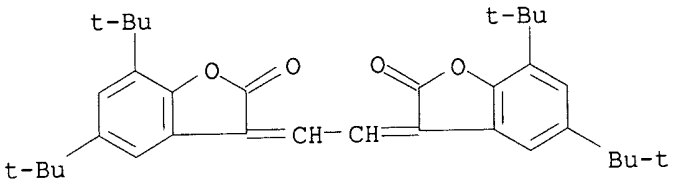
RN 293750-58-0 HCA
CN 2,3-Benzofurandione, 5-butyl-7-methoxy-, 3-[(5-butyl-7-methoxy-2-oxo-3(2H)-benzofuranylidene)hydrazone] (9CI) (CA INDEX NAME)



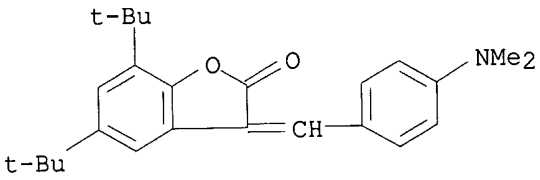
RN 293750-69-3 HCA
CN 2(3H)-Benzofuranone, 5-(1,1-dimethylethyl)-3-[(2-hydroxy-1-naphthalenyl)imino]-7-methoxy- (9CI) (CA INDEX NAME)



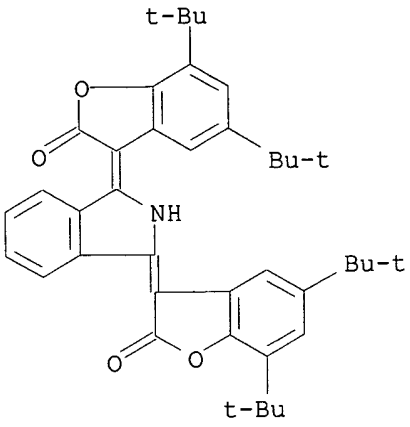
RN 293750-71-7 HCA
CN 2(3H)-Benzofuranone, 3,3'-(1,2-ethanediylidene)bis[5,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



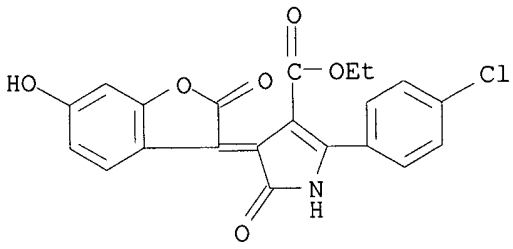
RN 293750-72-8 HCA
CN 2(3H)-Benzofuranone, 3-[[4-(dimethylamino)phenyl]methylene]-5,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



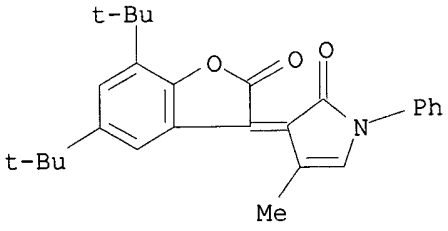
IT **293750-24-0P 293750-62-6P 293750-63-7P**
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(violet; prepn. of benzofuranone derivs. as styryl dye analogs)
RN 293750-24-0 HCA
CN 2(3H)-Benzofuranone, 3,3'-(1H-isoindole-1,3(2H)-diylidene)bis[5,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



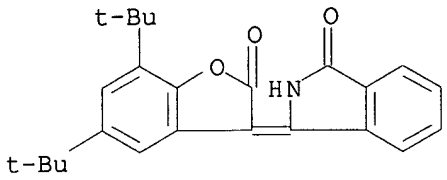
RN 293750-62-6 HCA
CN 1H-Pyrrole-3-carboxylic acid, 2-(4-chlorophenyl)-4,5-dihydro-4-(6-hydroxy-2-oxo-3(2H)-benzofuranylidene)-5-oxo-, ethyl ester (9CI) (CA INDEX NAME)



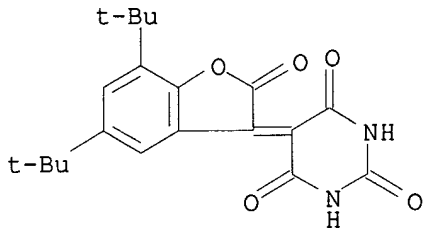
RN 293750-63-7 HCA
CN 2H-Pyrrol-2-one, 3-[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]-1,3-dihydro-4-methyl-1-phenyl- (9CI) (CA INDEX NAME)



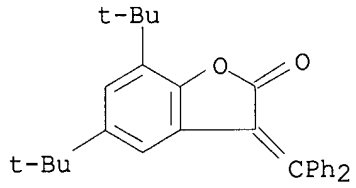
IT **253586-34-4P 293750-15-9P 293750-21-7P**
293750-28-4P 293750-29-5P 293750-31-9P
293750-33-1P 293750-34-2P 293750-35-3P
293750-37-5P 293750-38-6P 293750-39-7P
293750-41-1P 293750-43-3P 293750-44-4P
293750-66-0P 293750-67-1P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(yellow; prepn. of benzofuranone derivs. as styryl dye analogs)
RN 253586-34-4 HCA
CN 1H-Isoindol-1-one, 3-[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]-2,3-dihydro- (9CI) (CA INDEX NAME)



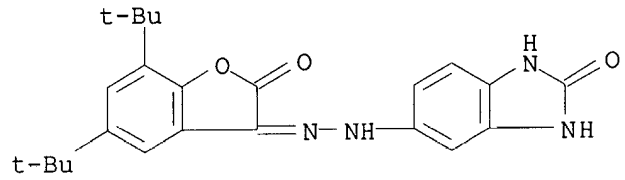
RN 293750-15-9 HCA
CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]- (9CI) (CA INDEX NAME)



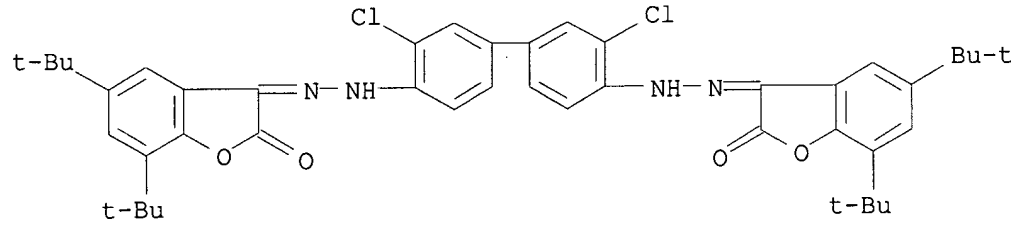
RN 293750-21-7 HCA
CN 2(3H)-Benzofuranone, 5,7-bis(1,1-dimethylethyl)-3-(diphenylmethylene)- (9CI) (CA INDEX NAME)



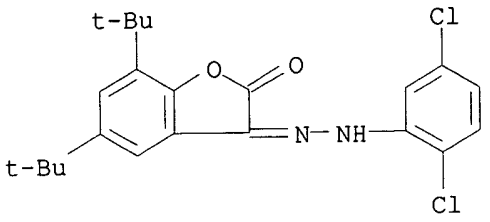
RN 293750-28-4 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)hydrazone] (9CI) (CA INDEX NAME)



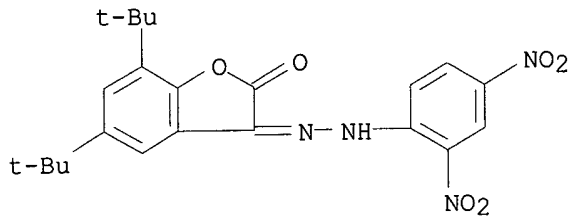
RN 293750-29-5 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3,3'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)dihydrazone] (9CI) (CA INDEX NAME)



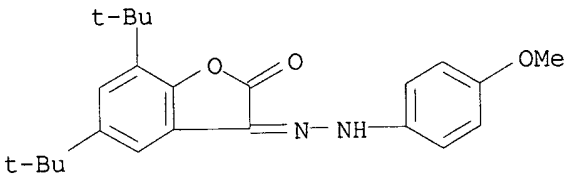
RN 293750-31-9 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[(2,5-dichlorophenyl)hydrazone] (9CI) (CA INDEX NAME)



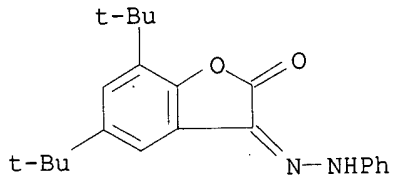
RN 293750-33-1 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[(2,4-dinitrophenyl)hydrazone] (9CI) (CA INDEX NAME)



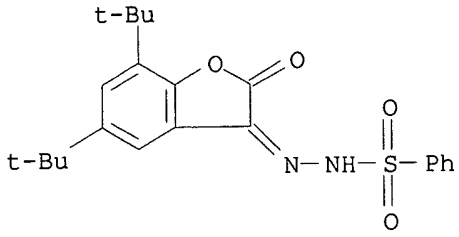
RN 293750-34-2 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[(4-methoxyphenyl)hydrazone] (9CI) (CA INDEX NAME)



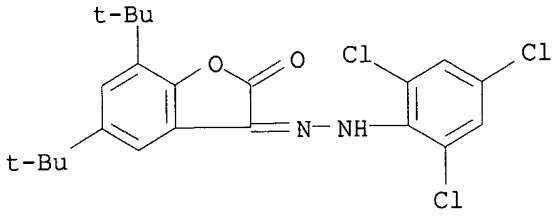
RN 293750-35-3 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-(phenylhydrazone) (9CI) (CA INDEX NAME)



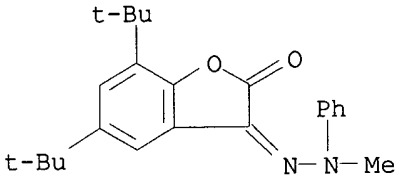
RN 293750-37-5 HCA
CN Benzenesulfonic acid, [5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]hydrazide (9CI) (CA INDEX NAME)



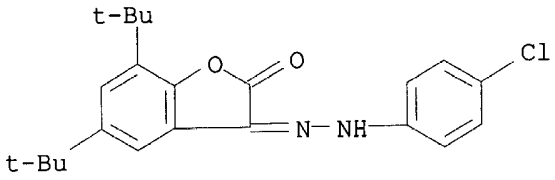
RN 293750-38-6 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[(2,4,6-trichlorophenyl)hydrazone] (9CI) (CA INDEX NAME)



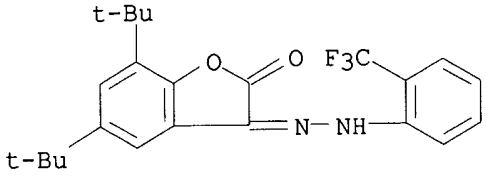
RN 293750-39-7 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-(methylphenylhydrazone) (9CI) (CA INDEX NAME)



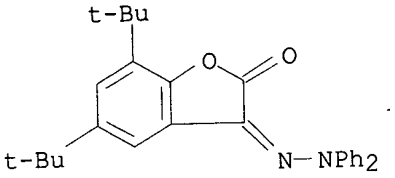
RN 293750-41-1 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[(4-chlorophenyl)hydrazone] (9CI) (CA INDEX NAME)



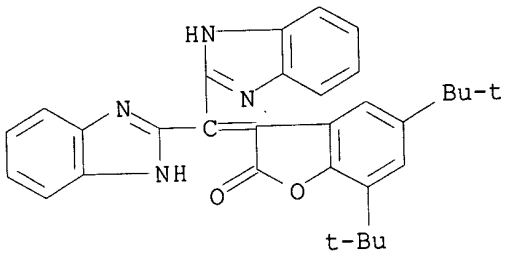
RN 293750-43-3 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-[[2-(trifluoromethyl)phenyl]hydrazone] (9CI) (CA INDEX NAME)



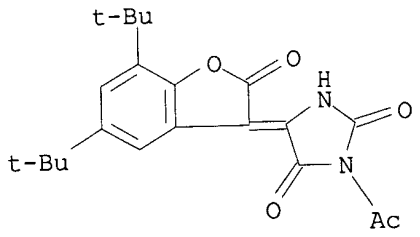
RN 293750-44-4 HCA
CN 2,3-Benzofurandione, 5,7-bis(1,1-dimethylethyl)-, 3-(diphenylhydrazone) (9CI) (CA INDEX NAME)



RN 293750-66-0 HCA
CN 2(3H)-Benzofuranone, 3-[bis(1H-benzimidazol-2-yl)methylene]-5,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



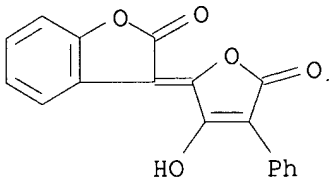
RN 293750-67-1 HCA
CN 2,4-Imidazolidinedione, 3-acetyl-5-[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]- (9CI) (CA INDEX NAME)



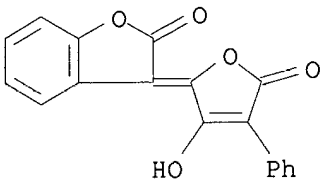
=> d L41 1,10,20,30,30-41 cbib abs hitstr (same compound)

L41 ANSWER 1 OF 30 HCA COPYRIGHT 2003 ACS
121:199918 Analysis of secondary metabolites from lichen by high performance liquid chromatography with a photodiode array detector. Yoshimura, Isao; Kinoshita, Yasuhiro; Yamamoto, Yoshikazu; Huneck, Siegfried; Yamada, Yasuyuki (Kochi Gakun College, Kochi, 780, Japan). Phytochemical Analysis, 5(4), 197-205 (English) **1994**. CODEN: PHANEL. ISSN: 0958-0344.
AB Secondary metabolites from Lichen, mainly phenolic compds., have been analyzed and identified using high performance liq. chromatog. with a photodiode array detector. Components of lichen thalli were detected by characteristic UV spectra and relative retention times. Some new minor components have been found in several lichens.

IT **10091-92-6**, Calycin
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)
(secondary metabolites from Lichen anal. by HPLC with photodiode array detector)
RN 10091-92-6 HCA
CN 2(3H)-Benzofuranone, 3-(3-hydroxy-5-oxo-4-phenyl-2(5H)-furanylidene)-(9CI) (CA INDEX NAME)

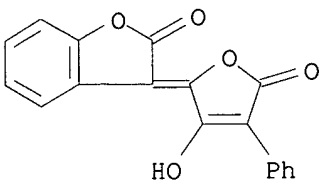


L41 ANSWER 10 OF 30 HCA COPYRIGHT 2003 ACS
76:123969 Isolation and investigation of substances contained in some lichens. Soviar, Karol (Dep. Pharm. Chem., Fac. Pharm., Bratislava, Czech.). Acta Facultatis Pharmaceuticae Universitatis Comenianae, 20, 27-56 (German) **1971**. CODEN: AFPCAG. ISSN: 0301-2298.
AB The following compds. were isolated: from Lepraria latebrarum roccellic acid (2-dodecyl-3-methylsuccinic acid) (I) and lepraric acid (II); from L. aeruginosa (.+-.)-usnic acid (III), (+)-protolichesteric acid (IV), atranorin (V), and I (cf. CA 70: 44812r); from L. flava (+)-III, vulpinic acid, I, and calycin (cf. CA 70: 65157w). Treatment of II with NaBH4 in tetrahydrofuran gave cis- and trans-.beta.-methylglutaconic acid (VI) and eugenitin (cf. CA 67: 90607t), while cleavage with NaBH4 in MeOH led to VI and 5-hydroxy-7-methoxy-6-methyl-2-methoxymethylchromenone (cf. CA 73: 109624g). II, IV, and V showed highest antimicrobial activity; I was inactive.
IT **10091-92-6**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Lepraria)
RN 10091-92-6 HCA
CN 2(3H)-Benzofuranone, 3-(3-hydroxy-5-oxo-4-phenyl-2(5H)-furanylidene)-(9CI) (CA INDEX NAME)

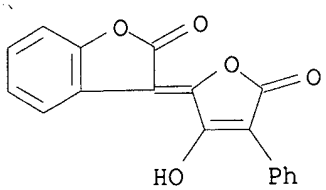


L41 ANSWER 20 OF 30 HCA COPYRIGHT 2003 ACS
66:52932 Lichen substances and systematics of the lobate types of the genus Lecanora in the Arctic. Eigler, G.; Poelt, J. (Univ. Munich, Munich, Germany). Oesterreichisches Botanisches Wochenblatt, 112(3), 285-94 (German) **1965**. CODEN: OBZEAS.
AB Usnic acid was the major physiol. active ingredient found chromatographically in exts. of 27 species of Lecanora and 10 species of Squamarina. Pulvinic anhydride and calycine were found in Candelariella medians and gyrophoric acid in Placopsis gelida. 13 references.
IT **10091-92-6**

RL: BIOL (Biological study)
(in lichens, taxonomy and)
RN 10091-92-6 HCA
CN 2(3H)-Benzofuranone, 3-(3-hydroxy-5-oxo-4-phenyl-2(5H)-furanylidene)-(9CI) (CA INDEX NAME)



L41 ANSWER 30 OF 30 HCA COPYRIGHT 2003 ACS
45:12218 Original Reference No. 45:2153i,2154a-d Antibiotics from lichens in therapy. Klosa, Josef (Erfurt, Germany). Medizinische Monatsschrift, 4, 816-20 (Unavailable) **1950**. CODEN: MEMOAQ. ISSN: 0025-8474.
AB cf. Pharmazie 5, 289(1950). Evosin II or parmycin is prepd. from Parmelia physodes and consists mainly of physodic and physodalic acid. The m.p. of substances newly prepd. from lichens is reported together with the antibiotic potency (Mycobacterium tuberculosis, active 1:1000+, 1:10,000++, 1:1,000,000 and higher +++) as follows: antranoric acid, m. 190-4.degree., from Lecoraceae, ++; atraric acid, m. 140.degree., from Cladoniaceae, ++; calycin, m. 240.degree., Calyciaceae from oaks, +; caperatic acid, m. 132.degree., Parmeliaceae, ++; caperin, m. 240.degree., Parmeliaceae from oaks, +; caperidin, m. 263.degree., Parmeliaceae from oaks, ++; capraric or physodalic acid, m. 260.degree., Parmeliaceae, +++; evernic acid, m. 191.degree., Ramalina pollinaris and Evernia prunastri, +++; lecanoric acid, m. 167.degree., Usnaeceae, ++; physodic acid, m. 202.degree., +++; pikrolichenic acid, m. 181.degree., Perussiaceae from beech, +++; ramalic acid, m. 180.degree., Rama lina farnicea, +++; salacinic acid, m. 260.degree., Pertussaria amara (beech and linden)++; usninic acid, m. 200.degree., from Parmeliaceae, Usnaceae, or Cladoniaceae, +++. The acids are phenolcarboxylic acids interconnected by O bridges. Evosin is sol. in H2O at a pH 7 to 7.5, better in a mixt. of EtOH and Me2CO. Oral doses of 4 g. in rats and of 15 g. in man given for several days are nontoxic. Daily intravenous doses of 20 mg. may cause fever. Evernic, usninic, physodic, caperatic, and evernuric acids and parmelin, dissolved in oil, were toxic in guinea pigs from 35 mg. on. Evosin was of value in chronically infected wounds (especially when combined with glycine or urea) and against many fungi, scabies, and worm infestations.
IT **10091-92-6**, Calycin
(prepn. of)
RN 10091-92-6 HCA
CN 2(3H)-Benzofuranone, 3-(3-hydroxy-5-oxo-4-phenyl-2(5H)-furanylidene)-(9CI) (CA INDEX NAME)



L41 ANSWER 30 OF 30 HCA COPYRIGHT 2003 ACS

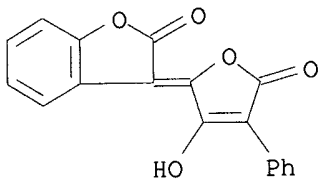
45:12218 Original Reference No. 45:2153i,2154a-d Antibiotics from lichens in therapy. Klosa, Josef (Erfurt, Germany). Medizinische Monatsschrift, 4, 816-20 (Unavailable) **1950**. CODEN: MEMOAQ. ISSN: 0025-8474.

AB cf. Pharmazie 5, 289(1950). Evosin II or parmycin is prepd. from Parmelia physodes and consists mainly of physodic and physodalic acid. The m.p. of substances newly prepd. from lichens is reported together with the antibiotic potency (Mycobacterium tuberculosis, active 1:1000+, 1:10,000++, 1:1,000,000 and higher +++) as follows: antranoric acid, m. 190-4.degree., from Lecoraceae, ++; atraric acid, m. 140.degree., from Cladoniaceae, ++; calycin, m. 240.degree., Calyciaceae from oaks, +; caperatic acid, m. 132.degree., Parmeliaceae, ++; caperin, m. 240.degree., Parmeliaceae from oaks, +; caperidin, m. 263.degree., Parmeliaceae from oaks, ++; capraric or physodalic acid, m. 260.degree., Parmeliaceae, +++; evernic acid, m. 191.degree., Ramalina pollinaris and Evernia prunastri, +++; lecanoric acid, m. 167.degree., Usnaeceae, ++; physodic acid, m. 202.degree., +++; pikrolichenic acid, m. 181.degree., Perussiaceae from beech, +++; ramalic acid, m. 180.degree., Rama lina farnicea, +++; salacinic acid, m. 260.degree., Pertussaria amara (beech and linden)++; usninic acid, m. 200.degree., from Parmeliaceae, Usnaceae, or Cladoniaceae, +++. The acids are phenolcarboxylic acids interconnected by O bridges. Evosin is sol. in H2O at a pH 7 to 7.5, better in a mixt. of EtOH and Me2CO. Oral doses of 4 g. in rats and of 15 g. in man given for several days are nontoxic. Daily intravenous doses of 20 mg. may cause fever. Evernic, usninic, physodic, caperatic, and evernuric acids and parmelin, dissolved in oil, were toxic in guinea pigs from 35 mg. on. Evosin was of value in chronically infected wounds (especially when combined with glycine or urea) and against many fungi, scabies, and worm infestations.

IT **10091-92-6**, Calycin
(prepn. of)

RN 10091-92-6 HCA

CN 2(3H)-Benzofuranone, 3-(3-hydroxy-5-oxo-4-phenyl-2(5H)-furanylidene)- (9CI) (CA INDEX NAME)

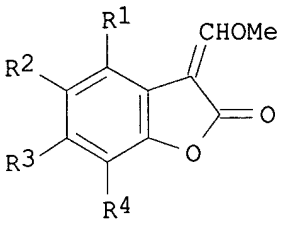


=> d L47 1,5,10,20,25,30,35,41 cbib abs hitstr Answers not close to applications cmpds.

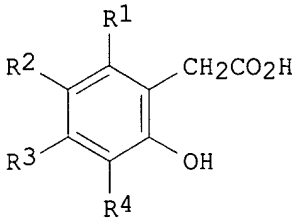
L47 ANSWER 1 OF 41 HCA COPYRIGHT 2003 ACS

129:41074 Preparation of 3-(.alpha.-methoxy)methylenebenzofuranones.. Jones, John David; Deboos, Gareth Andrew; Wilkinson, Paul; Cox, Brian Geoffrey; Fielden, Jan Michael (Zeneca Ltd., UK). U.S. US 5760250 A **19980602**, 15 pp., Division of U. S. Ser. No. 116,438, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1995-475282 19950607. PRIORITY: US 1991-788078 19911105; US 1993-116438 19930903.

GI



I



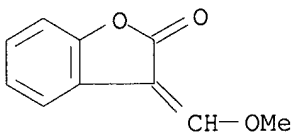
II

AB Title compds. (I; R1-R4 = H, halogen, alkyl, alkoxy, AcO, acyl), were prepd. by treating the corresponding unsubstituted benzofuranones with (MeO)3CH or with a dimethoxymethyl carboxylate or by cyclization of phenylacetates (II; R1-R4 as above) followed by reaction with (MeO)3CH or a dimethoxymethyl carboxylate, or by treatment of II with an acid anhydride and (MeO)3CH at 20-250.degree.. Thus, benzofuran-2(3H)-one, (MeO)3CH, and AcOH were heated at 100-105.degree. for 12 h to give 3-(.alpha.-methoxy)methylenebenzofuran-2-(3H)-one.

IT **40800-90-6P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 3-(.alpha.-methoxy)methylenebenzofuranones)

RN 40800-90-6 HCA

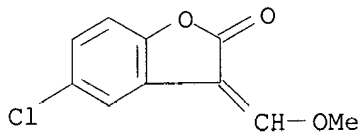
CN 2(3H)-Benzofuranone, 3-(methoxymethylene)- (9CI) (CA INDEX NAME)



IT **143230-44-8P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of 3-(.alpha.-methoxy)methylenebenzofuranones)

RN 143230-44-8 HCA

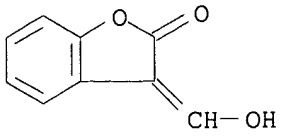
CN 2(3H)-Benzofuranone, 5-chloro-3-(methoxymethylene)- (9CI) (CA INDEX NAME)



IT **70450-82-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 3-(.alpha.-methoxy)methylenebenzofuranones)

RN 70450-82-7 HCA

CN 2(3H)-Benzofuranone, 3-(hydroxymethylene)- (9CI) (CA INDEX NAME)



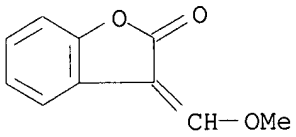
L47 ANSWER 5 OF 41 HCA COPYRIGHT 2003 ACS
125:283580 Allergic contact dermatitis from 3-(.alpha.-methoxy) methylenebenzofuran-2(3H)-one (MBF) and .alpha.-chloro-4-fluoroacetophenone (CFAP) in chemical process workers. Boffa, M. J.; Heron, R. J. L.; Wilkinson, S. M.; Beck, M. H. (School Medicine, University Manchester, Manchester, M60 9EP, UK). Contact Dermatitis, 34(6), 434-435 (English) **1996**. CODEN: CODEDG. ISSN: 0105-1873. Publisher: Munksgaard.

AB The authors report 2 cases of allergic contact dermatitis to MBF in chem. process workers, one of whom was also sensitized to CFAP.

IT **40800-90-6**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(allergic contact dermatitis from 3-(.alpha.-methoxy) methylenebenzofuran-2(3H)-one (MBF) and .alpha.-chloro-4-fluoroacetophenone (CFAP) in chem. process workers)

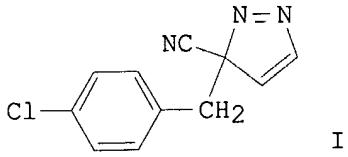
RN 40800-90-6 HCA

CN 2(3H)-Benzofuranone, 3-(methoxymethylene)- (9CI) (CA INDEX NAME)



L47 ANSWER 10 OF 41 HCA COPYRIGHT 2003 ACS
115:114410 Effect of electron-withdrawing groups on the thermal ring opening of 3H-pyrazoles to diazoalkenes. Nakano, Yoshihiko; Hamaguchi, Masashi; Nagai, Toshikazu (Coll. Gen. Educ., Osaka Univ., Toyonaka, 560, Japan). Journal of Chemical Research, Synopses (7), 170-1 (English) **1991**. CODEN: JRPSDC. ISSN: 0308-2342.

GI



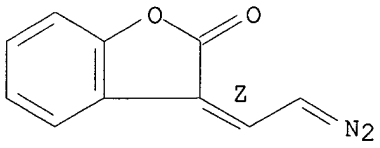
I

AB 3-Cyano-3H-pyrazoles, bearing a cyano, a p-chlorophenyl, or a p-chlorobenzyl group at C-3, e.g. I, generated from elimination reaction of the corresponding dihydropyrazoles with a leaving group such as a chlorine or p-chlorobenzoyloxy group, gave diazoalkene derivs., resulting from the ring-opening of the 3H-pyrazoles. 3-Methoxycarbonyl-3H-pyrazoles bearing a methoxycarbonyl, a p-chlorophenyl, or p-chlorobenzyl group at C-3, prepd. in a similar manner, gave mainly 1-methoxycarbonyl-1H-pyrazole derivs., resulting from migration of the 3-methoxycarbonyl group to the

adjacent nitrogen within the generated 3H-pyrazoles. Treatment of 3H-pyrazoles and 5-substituted 1-methoxycarbonyl-1H-pyrazoles with triethylamine gave 3-substituted 1-methoxycarbonyl-1H-pyrazoles, resulting from migration of the methoxycarbonyl group to the remote nitrogen.

IT **135641-98-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 135641-98-4 HCA
CN 2(3H)-Benzofuranone, 3-(diazoethylidene)-, (Z)- (9CI) (CA INDEX NAME)

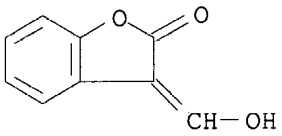
Double bond geometry as shown.



L47 ANSWER 20 OF 41 HCA COPYRIGHT 2003 ACS
91:4692 .beta.,.beta.-Diacylenamines and -enoles, III. Formylation of CH2-acidic compounds via the anilinomethylene derivatives. Wolfbeis, Otto S.; Junek, Hans (Inst. Org. Chem., Univ. Graz, Graz, A-8010, Austria). Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie, 34B(2), 283-9 (English) **1979**. CODEN: ZNBAD2. ISSN: 0340-5087.

AB Three component condensation of active methylene compds. with aniline and trialkyl orthoformate gives anilinomethylene-1,3-dicarbonyls, which can be hydrolyzed with aq. K2CO3, KOH or HCl, depending on the sensitivity of the hydroxymethylene deriv. thus formed. The reaction sequence is generally applicable: cyclohexane-1,3-diones, pyrimidine-3,5-diones (including barbituric acids), pyrazolones and pyrazoline-3,5-diones, indan-1,3-dione, (thio)phthalide, indoxyl, oxindole, anthrone, 2,6- and 2,7-dihydroxynaphthalene, and pentane-2,4-dione were formylated. Using orthoacetate or orthopropionate, tetronic acid, pyrazolones and pyrazolin-3,5-diones, resp., could also be acylated by this method.

IT **70450-82-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 70450-82-7 HCA
CN 2(3H)-Benzofuranone, 3-(hydroxymethylene)- (9CI) (CA INDEX NAME)



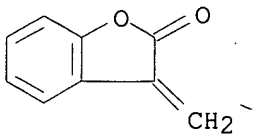
L47 ANSWER 25 OF 41 HCA COPYRIGHT 2003 ACS
80:90407 Electroplating of nickel. Brown, Henry (Oxy Metal Finishing Corp.). U.S. US 3770730 **19731106**, 3 pp. Division of U.S. 3,663,378 (CA 77;108822y). (English). CODEN: USXXAM. APPLICATION: US 1972-223754 19720204.

GI For diagram(s), see printed CA Issue.

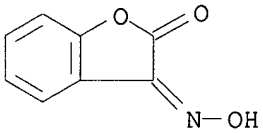
AB Same disclosure as in the earlier patent, but here the brighteners (e.g. I) are claimed as new chem. compds.

IT **51493-55-1**

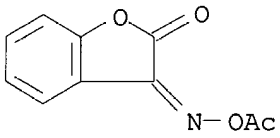
RL: PRP (Properties)
(in electroplating, of nickel, brightener)
RN 51493-55-1 HCA
CN 2(3H)-Benzofuranone, 3-methylene- (9CI) (CA INDEX NAME)



L47 ANSWER 30 OF 41 HCA COPYRIGHT 2003 ACS
78:124421 Antiviral substances. Carbamoyloximino derivatives of isatin and its heterocyclic analogs. Giannella, M.; Pigini, M. (Ist. Chim. Farm. Chim. Org., Univ. Camerino, Camerino, Italy). Farmaco, Edizione Scientifica, 28(2), 157-63 (Italian) **1973**. CODEN: FRPSAX. ISSN: 0430-0920.
GI For diagram(s), see printed CA Issue.
AB Carbamoyloximino heterocycles I(X = S, NH; R = Me, Ph) and II (Y = O, NH, NMe, NEt; R = Me, Ph) were prepd. by treating the corresponding oximines with RNCO 1-Methyl-3-(N-methyl) thiocarbamoyloximinoisatin (III) was similarly obtained with MeNCS. I(X = S, NH; R = Ph), II (Y = NMe, NEt; R = Ph; Y = NEt, R = Me) and III showed antiviral activity in vitro, but not in vivo. I(X = S, NH; R = Ph) and II (Y = NH, NEt, R =Ph) inhibited gastric secretion at 50 mg/kg in rats, but with toxic side effects.
IT **17892-65-8P 40785-36-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 17892-65-8 HCA
CN 2,3-Benzofurandione, 3-oxime (8CI, 9CI) (CA INDEX NAME)



RN 40785-36-2 HCA
CN 2,3-Benzofurandione, 3-(O-acetyloxime) (9CI) (CA INDEX NAME)



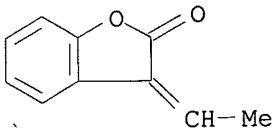
L47 ANSWER 35 OF 41 HCA COPYRIGHT 2003 ACS
71:70668 Ether cleavage with magnesium. Direct preparation of allylmagnesium phenolates. Maercker, Adalbert (Univ. Erlangen-Nuernberg, Erlangen, Fed. Rep. Ger.). Journal of Organometallic Chemistry, 18(2), 249-62 (German) **1969**. CODEN: JORCAI. ISSN: 0022-328X.
AB Allyl phenyl ether and some of its derivs. are cleaved by metallic Mg whereby allylmagnesium phenoxides are formed in excellent yields. Wurtz type coupling products, i.e., biallyl compds., are only observed working in very concd. solns. The corresponding cleavage of 2H-chromene yields an

interesting cyclic allylmagnesium phenoxide.

IT **4412-04-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 4412-04-8 HCA

CN 2(3H)-Benzofuranone, 3-ethylidene- (8CI, 9CI) (CA INDEX NAME)



L47 ANSWER 41 OF 41 HCA COPYRIGHT 2003 ACS

50:12302 Original Reference No. 50:2561b-i,2562a-f The rearrangement of 2-acetyl- and 2-benzoylcoumarone oxime p-toluenesulfonates. Geissman, T. A.; Armen, Ardy (Univ. of California, Los Angeles). Journal of the American Chemical Society, 77, 1623-7 (Unavailable) **1955**. CODEN: JACSAT. ISSN: 0002-7863.

GI For diagram(s), see printed CA Issue.

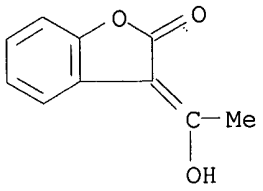
AB The rearrangement of the tosylate (I) of 2-acetylcoumarone oxime (II) to 2-methyl-3-chromonol (III) (cf. Vargha, et al., C.A. 44, 2973d) has been confirmed. A structure for the so-called acetal (IV) formed in the reaction has been proposed; it appears likely that IV has structure V. The rearrangement of 2-benzoylcoumarone oxime (VI) tosylate (VII) yielded flavonol (VIII) and 2-benzoyl-3-coumaranone (IX). New syntheses have been described for 2-acylcoumaranones; and 3-acetyl-2-coumaranone (X) has been described for the 1st time, correcting an earlier report of its prepn. by Pfeiffer and Enders (C.A. 45, 9046d). I prepd. and treated with MeOH by the method of Vargha, et al. (loc. cit.), yielded III, m. 179-81.degree., and IV, b4 122-7.degree., nD25 1.5142. Dry Me2CO (100 cc.), 75 g. K2CO3, 50 g. o-HOC6H4CO2Me, and 30.4 g. AcCH2Cl heated 5 hrs. on the steam bath, the mixt. cooled, dild. with H2O, and extd. 3 times with Et2O, the aq. phase acidified, and the cryst. ppt. (8.0 g.) recrystd. from ligroine and dil. EtOH gave 2-acetylcoumaranone (Xa), m. 90-1.degree.; it gave an olive-green color with FeCl3 in dil. aq. NaHCO3; an Et2O soln. treated with Cu(OAc)2 gave a Cu complex; it gave a blood-red 2,4-dinitrophenylhydrazone. o-HOC6H4COCH2Ac (XI) (2.0 g.) in 200 cc. CHCl3, contg. 2 g. K2CO3 treated dropwise with stirring at 0.degree. with 1.8 g. Br in 40 cc. CHCl3, the colorless mixt. kept 0.5 hr. at 0.degree., refluxed 1 hr., filtered, and extd. with 5% aq. Na2CO3, and the aq. ext. acidified yielded 0.81 g. Xa, colorless crystals, m. 90-2.degree.. Xa treated with Ac2O and pyridine gave the acetate, m. 86-7.degree.. 2-Methylchromone (3.1 g.) (prepd. by the acid-catalyzed ring closure of XI) in 30 cc. C6H6 hydrogenated 22 hrs. at atm. pressure over 3.1 g. Pd-CaCO3, the mixt. filtered and evapd., the residual oil dissolved in 60 cc. abs. EtOH, 6 cc. AcOH, and 6 g. Girard reagent T, the soln. refluxed 1 hr., cooled, treated with 250 cc. ice cold H2O contg. 3.6 g. Na2CO3, the soln. extd. with Et2O, made 0.5N in HCl, kept 1 hr. at room temp., and extd. with Et2O yielded 1.74 g. VI. VI (0.74 g.) in 35 cc. boiling 95% EtOH treated alternately with shaking portionwise with 4.0 cc. AmONO and 20 cc. concd. HCl, the soln. allowed to stand 2 hrs., dild. with 100 cc. H2O and cooled gave 0.52 g. III, m. 178-80.degree.; it gave a violet-blue color with FeCl3. VI treated with AmONO under alk. conditions followed by hydrolysis of the intermediate isonitroso deriv. gave a somewhat poorer yield of III. IV (240 mg.) in 10 cc. EtOH and 10 cc. 2N H2SO4 refluxed 2 hrs. did not give any III, but the mixt. refluxed 3 days and then cooled gave 60 mg. III. IV did not give CHI3 with NaOI, nor CHBr3 with NaOBr.

IV (0.50 g.) in 15 cc. 48% HBr heated 1 hr. at 120.degree., the soln. cooled, dild. with 100 cc. H2O, and extd. with Et2O, the ext. shaken with N aq. NaOH, the basic soln. filtered and acidified, and the ppt. recrystd. from dil. EtOH gave 0.13 g. 2-methylcoumarone-3-carboxylic acid (XII), m. 190-1.degree. (from aq. EtOH). o-HOC6H4CH2CO2H (1.5 g.) and 4 cc. Ac2O heated 0.5 hr. in 30 cc. pyridine on the steam bath, the mixt. cooled, dild. with dil. HCl, and again cooled, the resulting solid (0.95 g.) dissolved in aq. NaHCO3, the soln. decolorized with Norite, filtered, and acidified, and the colorless ppt. recrystd. from aq. EtOH gave X, m. 133-4.degree.; it gave a deep blue color with FeCl3. X treated with CH2N2 in Et2O gave the Me ether, m. 125-6.degree.. X treated 2 hrs. with Ac2O and NaOAc gave the acetate, m. 114-16.degree.. Isocoumaranone (0.53 g.) in 10 cc. dry EtOAc treated with 0.10 g. NaH, the mixt. refluxed 1 hr., cooled, treated with 20 cc. dil. HCl, the Et2O layer extd. with aq. NaHCO3, and the aq. alk. ext. acidified gave 0.30 g. colorless compd., m. 155-6.degree., probably 3-o-hydroxy-phenylacetylisocoumaranone; it gave a deep blue color with FeCl3. 2-Methylcoumarone (13 g.) was converted to the 3-Br deriv. (XIII), b6 100-4.degree., nD20 1.5870. XIII (0.50 g.) in 10 cc. Et2O added at -78.degree. to 8 cc. 0.32M BuLi in 15 cc. Et2O, the mixt. treated after 2 min. with excess Dry Ice, warmed to room temp., and dild. with H2O, the Et2O layer washed twice with aq. NaHCO3, and the aq. ext. acidified gave XII, m. 190-1.degree.. 2-Benzoylcoumarone (20 g.) refluxed 2 hrs. with 18.8 g. NH2OH.HCl and 50.5 g. KOH in aq. EtOH, the mixt. dild. with H2O and cooled, and the cryst. deposit recrystd. from aq. AcOH gave 18.2 g. VI, m. 128-9.5.degree.. p-MeC6H4SO2Cl (XIV) (0.46 g.), 0.50 g. VI, and 1 cc. dry pyridine kept 1 hr. at room temp., the mixt. dild. with Et2O, the Et2O soln. washed 3 times with dil. H2SO4, twice with 2N NaOH, and twice with H2O, dried, and evapd. to dryness in vacuo at room temp., the oily residue dissolved in EtOH, and the soln. dild. to beginning crystn. gave VII, m. 109-10.degree.. VII (14.35 g.), m. 102-5.degree., gave in an attempted recrystn. from hot aq. EtOH coumarilanilide (XV), m. 151-4.degree.; the aq. alc. mother liquor extd. with Et2O, the ext. washed with dil. aq. NaOH, and the alk. soln. acidified gave 0.33 g. VIII, m. 167-8.degree.. Crude VII from 10 g. VI and 9.2 g. XIV in 20 cc. dry pyridine in Et2O soln. dild. with 200 cc. 80% aq. MeOH, the Et2O distd. off, the residual soln. refluxed 2 hrs., cooled, and extd. with Et2O, the ext. washed with 5% aq. NaHCO3, and the aq. alk. washing acidified yielded 40 mg. IX, m. 79-80.degree. (from aq. EtOH); it gave an olive-green color with FeCl3; the remaining Et2O soln. extd. with dil. aq. NaOH, and the alk. ext. acidified yielded 1.1 g. VIII, m. 166-7.degree. (from EtOH); the residual Et2O soln. dried and evapd., and the partially cryst. material (9.0 g.) recrystd. from EtOH gave 2.05 g. XV, m. 155-6.degree.; the EtOH mother liquor extd. with Et2O, a 50-cc. aliquot of the ext. (250 cc.) evapd., and the residual oil (1.15 g.) sapond. gave 0.27 g. coumarilic acid, m. 190-1.degree.; the residue from another 50-cc. aliquot distd. at 6 mm. and the resulting cryst. distillate (0.30 g.), b. below 190.degree., recrystd. from dil. EtOH gave Me coumarilate, m. 51-2.degree.. o-HOC6H4COCH2Bz (0.65 g.) and 0.8 g. dry K2CO3 in 50 cc. CHCl3 treated with stirring at 0.degree. with 0.44 g. Br in 10 cc. CHCl3, the mixt. refluxed 1 hr., cooled, and washed with N NaOH, the aq. alk. washings acidified, and the resulting ppt. recrystd. from aq. EtOH gave 0.37 g. 2-benzoylcoumaranone, m. 79-80.degree.; it gave an olive-green color with FeCl3.

IT **101012-55-9**, Crotonic acid, 3-hydroxy-2-(o-hydroxyphenyl)-, .gamma.-lactone
(prepn. of)

RN 101012-55-9 HCA

CN 2(3H)-Benzofuranone, 3-(1-hydroxyethylidene)- (9CI) (CA INDEX NAME)



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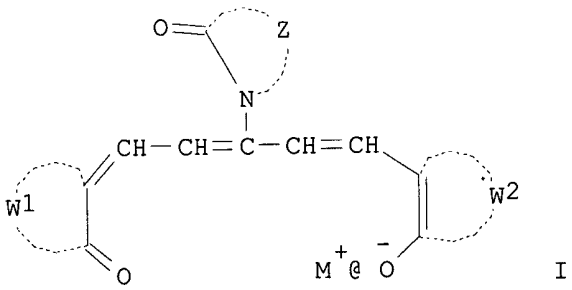
1,5,10,15,20,25,30,32,37,45,51,58,63,69,70,72,76,78,80,90,100,112,120,125,130,135,140,145,150,155,160-169 cbib abs hitstr

L50 ANSWER 1 OF 162 HCA COPYRIGHT 2003 ACS
134:49131 Oxonol compound, light-sensitive material and process for the synthesis of oxonol compound. Nishigaki, Junji; Deguchi, Yasuaki (Fuji Photo Film Co., Ltd., Japan). U.S. US 6159673 A 20001212, 72 pp., Cont.-in-part of U.S. Ser. No. 896,064, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1999-233444 19990120. PRIORITY: JP 1996-206527 19960717; JP 1996-235893 19960819; JP 1997-55315 19970310; US 1997-896064 19970717.
GI



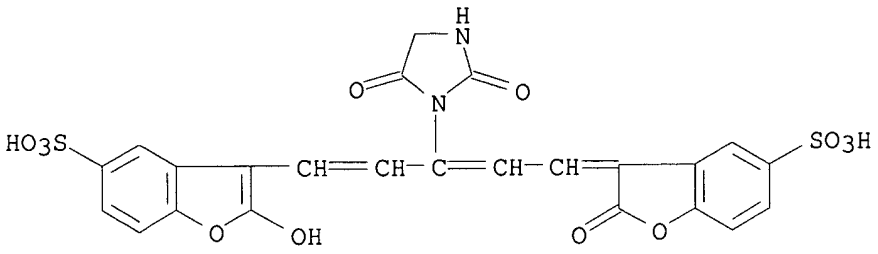
I

AB The invention relates to oxonol compds., a light-sensitive material contg. an oxonol compd. and a process for the synthesis of an oxonol compd. A light-sensitive material, particularly a silver halide photog. material, usually contains a dye which functions as an anti-irradn. dye, an antihalation dye or a filter dye that absorbs light of a specific wavelength. Oxonol compds. hav been known as representative photog. dyes. The oxonol compd. is represented by (I) in which Z is an at. group that forms a cyclic amide ring; each of W1 and W2 independently is an at. group that forms an acidic nucleus ring; and M is a cation. Other oxonol compds., a light-sensitive material contg. an oxonol compd. and a process for the synthesis of an oxonol compd. are also disclosed.

IT **202482-74-4P**
RL: NUU (Other use, unclassified); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(prepn. of methine dyes for oxonol as light-sensitive dye in silver halide photog. papers)

RN 202482-74-4 HCA
CN 5-Benzofuransulfonic acid, 3-[3-(2,5-dioxo-1-imidazolidinyl)-5-(2-hydroxy-

5-sulfo-3-benzofuranyl)-2,4-pentadienylidene]-2,3-dihydro-2-oxo-, tripotassium salt (9CI) (CA INDEX NAME)



●3 K

L50 ANSWER 5 OF 162 HCA COPYRIGHT 2003 ACS

129:275777 Chemical transformation of embelin through dimerization during preparation of a decoction. Kiuchi, Fumiyuki; Suzuki, Noriko; Fukumoto, Yumiko; Goto, Yoshihisa; Mitsui, Mariko; Tsuda, Yoshisuke (Faculty of Pharmaceutical Sciences, Kanazawa University, Kanazawa, 920-0934, Japan). Chemical & Pharmaceutical Bulletin, 46(8), 1225-1228 (English) **1998**. CODEN: CPBTAL. ISSN: 0009-2363. Publisher: Pharmaceutical Society of Japan.

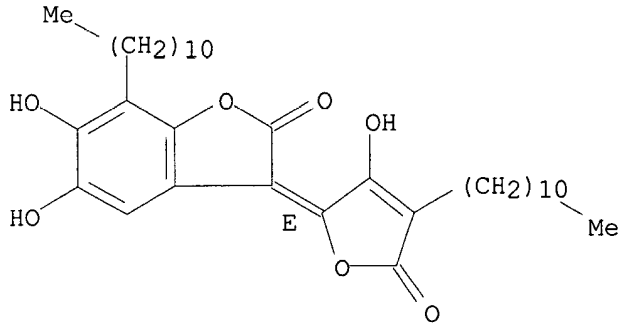
AB Embelin, a major constituent of Embelia ribes Burm. (Myrsinaceae) was transformed into different types of compds. through dimerization during prepn. of a decoction. Two of the products are proposed to have furanylidene benzofuranone and 1,4-dibenzofurandione skeletons on the basis of spectroscopic means. The transformation of embelin in boiling water is markedly accelerated by the presence of fatty acids.

IT **213822-01-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dimerization of embelin during prepn. of a decoction)

RN 213822-01-6 HCA

CN 2(3H)-Benzofuranone, 5,6-dihydroxy-3-(3-hydroxy-5-oxo-4-undecyl-2(5H)-furanylidene)-7-undecyl-, (3E)- (9CI) (CA INDEX NAME)

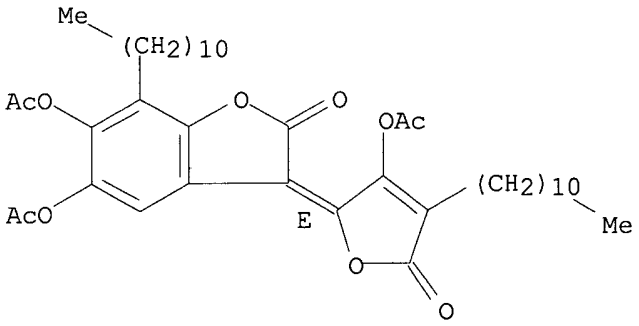
Double bond geometry as shown.



IT **213822-04-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(dimerization of embelin during prepn. of a decoction)

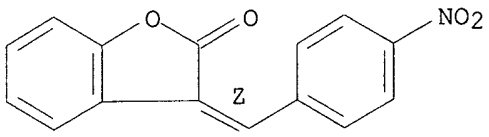
RN 213822-04-9 HCA
CN 2(3H)-Benzofuranone, 5,6-bis(acetyloxy)-3-[3-(acetyloxy)-5-oxo-4-undecyl-2(5H)-furanylidene]-7-undecyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



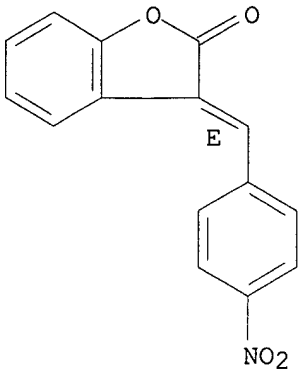
L50 ANSWER 10 OF 162 HCA COPYRIGHT 2003 ACS
128:217271 Regio- and stereochemistry of the [4+2] cycloaddition of 2-benzoyl-1,2-dihydroisoquinoline-1-carbonitrile tetrafluoroborate with (Z)- and (E)-3-arylidene-3H-benzofuranones. Msaddek, Moncef; Rammah, Mohamed; Ciamala, Kabula; Vebrel, Joel; Laude, Bernard (Departement de Chimie, Faculte des Sciences et Techniques, Universite du Centre, Monastir, 5000, Tunisia). Bulletin des Societes Chimiques Belges, 106(12), 825-831 (French) **1997**. CODEN: BSCBAG. ISSN: 0037-9646. OTHER SOURCES: CASREACT 128:217271. Publisher: Bulletin des Societes Chimiques Belges.
AB The reaction of 2-benzoyl-1,2-dihydroisoquinoline-1-carbonitrile tetrafluoroborate salt with 3-arylidene-2-(3H)-benzofuranones (Z or E) leads to a single spiro compd. irresp. of the double bond geometry of the starting olefin. In an acidic medium, the spiro compd. yields quant. a tetrasubstituted pyrrole. The regio- and stereochem. of the reaction was established from NMR data.
IT **118974-78-0 118974-79-1 119460-70-7 119460-71-8 202347-91-9 202347-92-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(regio- and stereochem. of the [4+2] cycloaddn. of benzoyldihydroisoquinolinecarbonitrile tetrafluoroborate with arylidenebenzofuranones)
RN 118974-78-0 HCA
CN 2(3H)-Benzofuranone, 3-[(4-nitrophenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



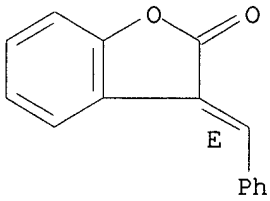
RN 118974-79-1 HCA
CN 2(3H)-Benzofuranone, 3-[(4-nitrophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



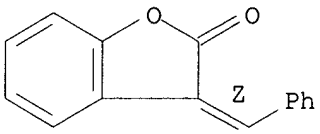
RN 119460-70-7 HCA
CN 2(3H)-Benzofuranone, 3-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



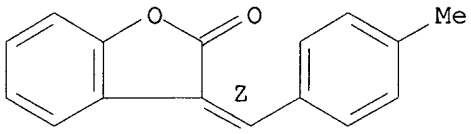
RN 119460-71-8 HCA
CN 2(3H)-Benzofuranone, 3-(phenylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



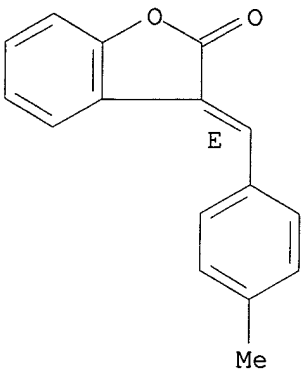
RN 202347-91-9 HCA
CN 2(3H)-Benzofuranone, 3-[(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



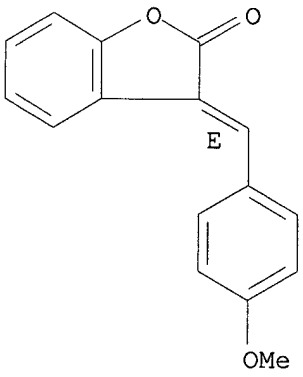
RN 202347-92-0 HCA
CN 2(3H)-Benzofuranone, 3-[(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



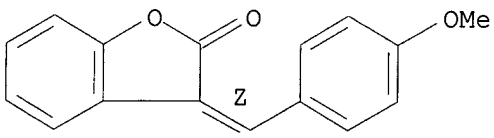
IT **59020-02-9P 59020-03-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regio- and stereochem. of the [4+2] cycloaddn. of benzoyldihydroisoquinolinecarbonitrile tetrafluoroborate with arylidenebenzofuranones)
RN 59020-02-9 HCA
CN 2(3H)-Benzofuranone, 3-[(4-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 59020-03-0 HCA
CN 2(3H)-Benzofuranone, 3-[(4-methoxyphenyl)methylene]-, (3Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L50 ANSWER 15 OF 162 HCA COPYRIGHT 2003 ACS
127:212447 The design and development of new thermally stable infrared active

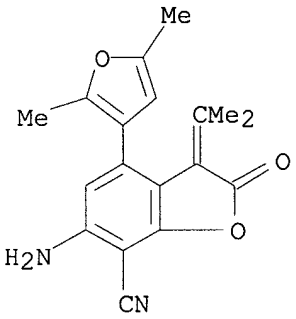
photochromic compounds. Heller, Harry G.; Koh, Kevin; Kose, Mamut; Rowles, Neil (Chemistry Department, University Wales, Cardiff, CF1 3TB, UK). Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals, 297, 73-80 (English) **1997**. CODEN: MCLCE9. ISSN: 1058-725X. Publisher: Gordon & Breach.

AB E-.beta.-dicyanomethylene-4-alkylidene-3-1-(substituted-3-furyl or 3-thienyl)ethylidene tetrahydrofuran-2-ones (prepd. by base-catalyzed condensation of the corresponding E-fulgides with malononitrile, followed by cyclization with acetyl chloride) undergo base-catalyzed cyclization to photochromic 3-alkylidene-6-amino-7-cyano(substituted-3-furyl or 3-thienyl)-2,3-dihydrobenzofuranones, which photocyclize to compds. having long wavelength absorption band maxima at ca. 750 nm. Charge transfer characteristics in the photochromes are essential for retention of arom. character in the annelated benzene ring.

IT **194602-38-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(design and development of new thermally stable IR active photochromic compds.)

RN 194602-38-5 HCA

CN 7-Benzofurancarbonitrile, 6-amino-4-(2,5-dimethyl-3-furanyl)-2,3-dihydro-3-(1-methylethylidene)-2-oxo- (9CI) (CA INDEX NAME)



L50 ANSWER 20 OF 162 HCA COPYRIGHT 2003 ACS

124:174934 Alkyl (E)- and (Z)-2,3-dibromopropenoates as precursors to 3-substituted alkyl (E)- and (Z)-2-bromopropenoates, 2,3-disubstituted alkyl (Z)- and (E)-propenoates and some heterocyclic compounds. Rossi, Renzo; Bellina, Fabio; Carpita, Adriano; Gori, Raffaele (Dip. Chim. Chim. Indu., Univ. Pisa, Pisa, I-56126, Italy). Gazzetta Chimica Italiana, 125(9), 381-92 (English) **1995**. CODEN: GCITA9. ISSN: 0016-5603. OTHER SOURCES: CASREACT 124:174934. Publisher: Societa Chimica Italiana.

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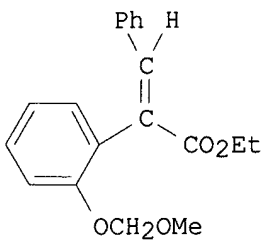
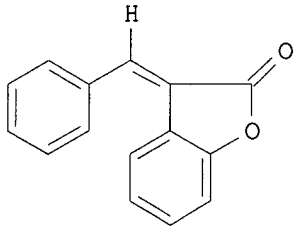


I



II

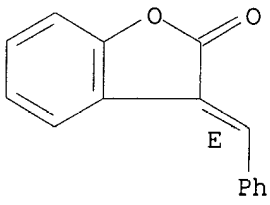
AB 3-(1-Alkynyl)- and 3-aryl-substituted alkyl (Z)- and (E)-2-bromopropenoates have been stereospecifically and regioselectively synthesized by Pd-catalyzed cross-coupling reactions between 1-alkynyl-zinc chlorides, arylzinc chlorides or aryltributylstannanes and alkyl (Z)- and (E)-2,3-dibromopropenoates, (Z)- and (E)-2, resp. The catalyst precursor consisting of a mixt. of Pd on carbon and 3.9 equiv of AsPh3 as well as that obtained by treatment of Pd(OAc)2 with 4 equiv of AsPh3 in THF at 60.degree. can conveniently replace Pd(PPh3)4 in the reactions between (Z)- or (E)-2 and aryl or 1-alkynylzinc halides. On the other hand, a representative alkyl (Z)-3-alkyl-2-bromopropenoate has been prepd. by reaction of a 9-alkyl-9-BBN deriv. with (Z)-2 in DMF soln., in the presence of K2CO3 and a catalytic quantity of PdCl2(dppf). Some applications demonstrate the synthetic utility of 3-aryl-substituted alkyl (Z)- and (E)-propenoates, (Z)- and (E)-4. Thus, Et (E)-2-bromo-3-[(2-methoxymethoxy)phenyl]propenoate, (E)-4e, represents a direct precursor to 3-bromocoumarin, 7, and compd. (Z)-8, which is obtained by acidic hydrolysis of (Z)4e, undergoes a Pd-catalyzed intramol. carbonylation reaction, which affords 3-ethoxycarbonylcoumarin, 9, in high yield. Moreover, treatment of compds. (Z)- and (E)-4 with organozinc or organotin derivs., in the presence of catalytic amts. of a suitable Pd catalyst, affords, stereospecifically and in satisfactory to excellent yields, (E)- and (Z)- trisubstituted .alpha.,.beta.-unsatd. esters, resp. (e.g. (E)- I), which cannot be easily prepd. in stereoisomerically pure form by classical procedures. One of these esters, i.e. compd. (E)-I, represents a direct precursor to an isoaurone, i.e. (E)-3-benzylidene-benzofuran-2-one, (E)-II. Finally, a representative stereo-defined unsym. 2,3-diaryl-disubstituted alkyl propenoate has been synthesized by a one-pot procedure involving two sequential palladium-catalyzed arylations of (Z)-2.

IT **119460-70-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(Pd-catalyzed cross-coupling reaction between alkyl- and aryl zinc chlorides and aryltributylstannanes and alkyl dibromopropenoates)

RN 119460-70-7 HCA

CN 2(3H)-Benzofuranone, 3-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

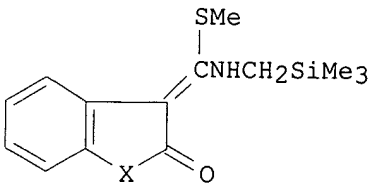
Double bond geometry as shown.



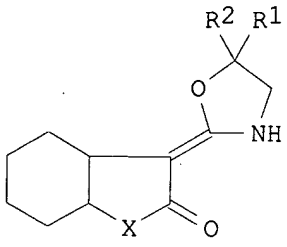
L50 ANSWER 25 OF 162 HCA COPYRIGHT 2003 ACS

122:160526 Synthesis and [3+2] cycloaddition reaction of 3-[(trimethylsilylmethylamino)(methylthio)]methylene-2-coumaranone and -1-methyloxindole: synthetic equivalent of heterocyclic alkylidene-azomethine ylide as a novel 1,3-dipolar reagent. Tominaga, Yoshinori; Takada, Satoshi; Kohra, Shinya (Faculty of Pharmaceutical of Sciences, Nagasaki Univ., Nagasaki, 852, Japan). Heterocycles, 39(1), 15-18 (English) **1994**. CODEN: HTCYAM. ISSN: 0385-5414. OTHER SOURCES: CASREACT 122:160526. Publisher: Japan Institute of Heterocyclic Chemistry.

GI



I



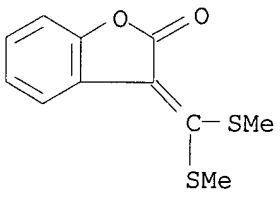
II

AB 3-[(Trimethylsilylmethylamino)(methylthio)]methylene-2-coumaranone (I, X = O) and -1-methyloxindole (I, X = NMe), readily prepd. by reaction of the corresponding bis(methylthio)methylene-heterocyclic compds. with H2NCH2SiMe3, were found to be synthetic equiv. of heterocyclic alkylideneazomethine ylides. Reaction of I with reactive hetero-dipolarophiles such as aldehydes and ketones in the presence of cesium fluoride gave 1,3-dipolar cycloadducts II [same X; R1 = H, Ph; R2 = (un)substituted Ph, 1-naphthyl, Me(CH2)3, PhCO] via the 1,3-elimination of (methylthio)trimethylsilane.

IT **161202-26-2P 161202-27-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and cycloaddn. reaction of [(trimethylsilylmethylamino)(methylthio)methylene]coumaranone and -methyloxindole)

RN 161202-26-2 HCA

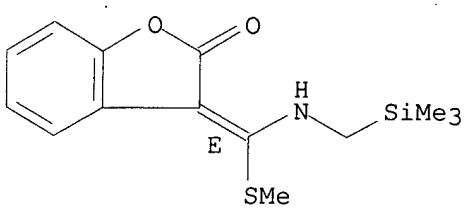
CN 2(3H)-Benzofuranone, 3-[bis(methylthio)methylene]- (9CI) (CA INDEX NAME)



RN 161202-27-3 HCA

CN 2(3H)-Benzofuranone, 3-[(methylthio)[[(trimethylsilyl)methyl]amino]methylene]-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

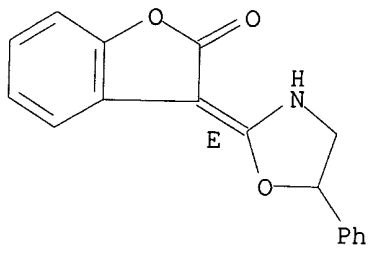


IT **161202-29-5P 161202-30-8P 161202-31-9P**
161202-32-0P 161202-33-1P 161202-34-2P

161202-35-3P 161202-36-4P 161202-37-5P
161202-38-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and cycloaddn. reaction of [(trimethylsilylmethylamino)(methylthio)methylene]coumaranone and -methyloxindole)

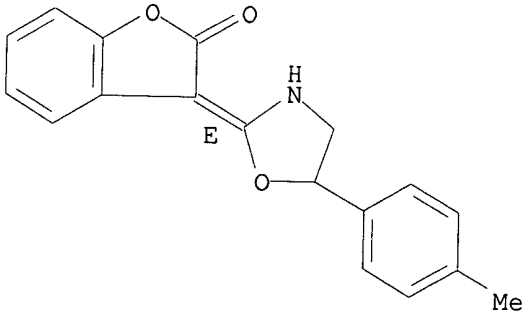
RN 161202-29-5 HCA
CN 2(3H)-Benzofuranone, 3-(5-phenyl-2-oxazolidinylidene)-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



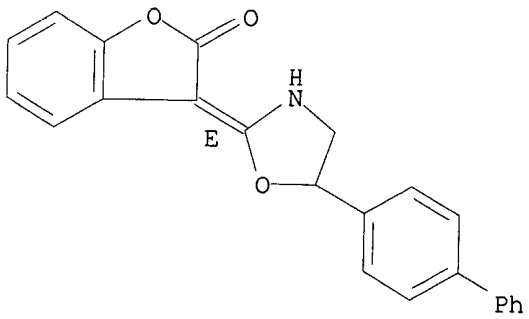
RN 161202-30-8 HCA
CN 2(3H)-Benzofuranone, 3-[5-(4-methylphenyl)-2-oxazolidinylidene]-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



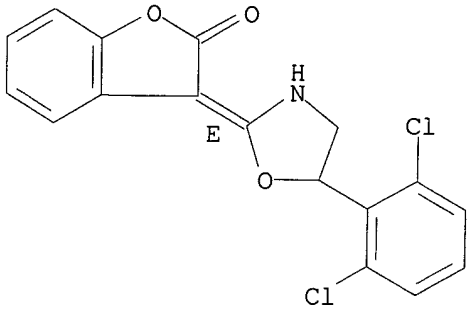
RN 161202-31-9 HCA
CN 2(3H)-Benzofuranone, 3-(5-[1,1'-biphenyl]-4-yl-2-oxazolidinylidene)-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



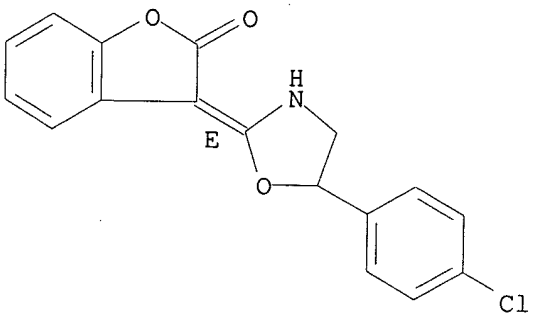
RN 161202-32-0 HCA
CN 2(3H)-Benzofuranone, 3-[5-(2,6-dichlorophenyl)-2-oxazolidinylidene]-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



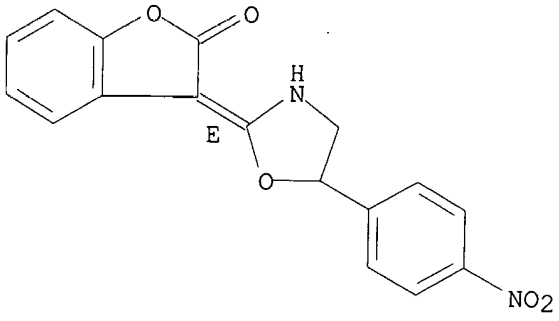
RN 161202-33-1 HCA
CN 2(3H)-Benzofuranone, 3-[5-(4-chlorophenyl)-2-oxazolidinylidene]-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



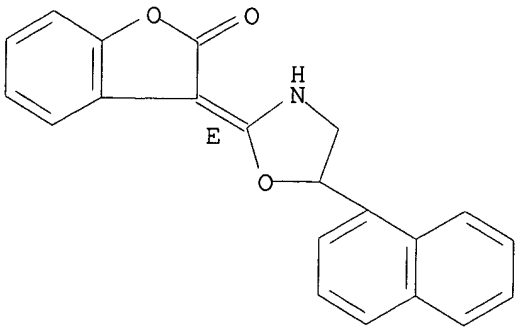
RN 161202-34-2 HCA
CN 2(3H)-Benzofuranone, 3-[5-(4-nitrophenyl)-2-oxazolidinylidene]-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



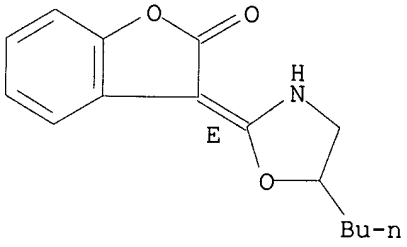
RN 161202-35-3 HCA
CN 2(3H)-Benzofuranone, 3-[5-(1-naphthalenyl)-2-oxazolidinylidene]-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



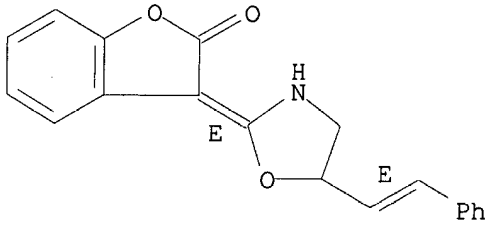
RN 161202-36-4 HCA
CN 2(3H)-Benzofuranone, 3-(5-butyl-2-oxazolidinylidene)-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



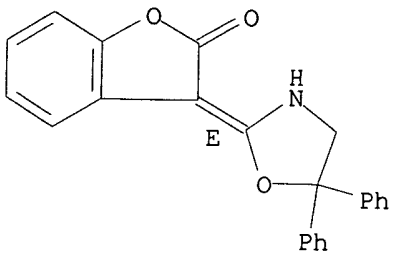
RN 161202-37-5 HCA
CN 2(3H)-Benzofuranone, 3-[5-[(1E)-2-phenylethenyl]-2-oxazolidinylidene]-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 161202-38-6 HCA
CN 2(3H)-Benzofuranone, 3-(5,5-diphenyl-2-oxazolidinylidene)-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



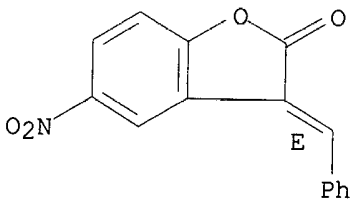
L50 ANSWER 30 OF 162 HCA COPYRIGHT 2003 ACS
118:186650 Fluxionate Lewis acidity of the zinc(2+) ion in carboxypeptidase A. Mock, William L.; Freeman, Dennis J.; Aksamawati, Mohammed (Dep. Chem., Univ. Illinois, Chicago, IL, 60607-7061, USA). Biochemical Journal, 289(1), 185-93 (English) **1993**. CODEN: BIJOAK. ISSN: 0306-3275.

AB Competitive Ki values for a series of phenol ring-substituted derivs. of .alpha.-(2-hydroxyphenyl)benzenepropanoic acid were ascertained by observing their influence on the catalytic hydrolysis of a peptide substrate by the Zn enzyme, carboxypeptidase A. The pH-dependence of Ki showed that binding was maximal between 2 pKa values: one was that of the phenol group of the inhibitor, and the other uniformly had a value of 6, the pKa of a Zn2+-bound water mol. on the enzyme in the absence of substrate or inhibitor. This was the dependence expected if phenolate binds to the Zn2+ displacing its bound H2O/HO-. A log-log plot of the dissocn. consts. for the productive forms of inhibitor plus enzyme vs. the acid dissocn. consts. of the phenolic residues in the inhibitors yielded a straight line with a slope of +0.76. This value indicated that the active-site metal has special capacity for dispersing neg. charge, such that which builds up on the O atom of a carboxamide group undergoing nucleophilic addn.

IT **147044-43-7P 147044-58-4P 147044-61-9P**
147044-62-0P 147044-64-2P 147044-66-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)

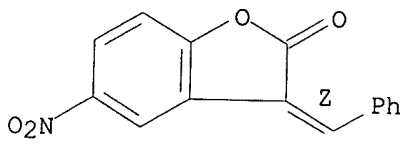
RN 147044-43-7 HCA
CN 2(3H)-Benzofuranone, 5-nitro-3-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

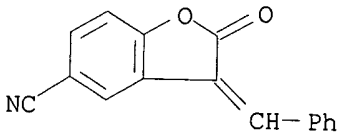


RN 147044-58-4 HCA
CN 2(3H)-Benzofuranone, 5-nitro-3-(phenylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

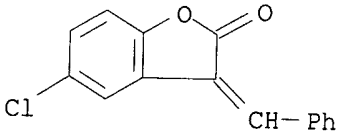
Double bond geometry as shown.



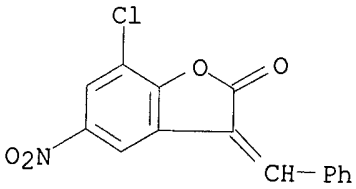
RN 147044-61-9 HCA
CN 5-Benzofurancarbonitrile, 2,3-dihydro-2-oxo-3-(phenylmethylene)- (9CI) (CA INDEX NAME)



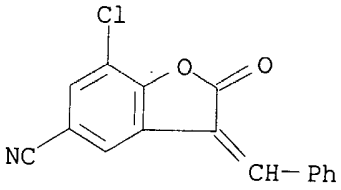
RN 147044-62-0 HCA
CN 2(3H)-Benzofuranone, 5-chloro-3-(phenylmethylene)- (9CI) (CA INDEX NAME)



RN 147044-64-2 HCA
CN 2(3H)-Benzofuranone, 7-chloro-5-nitro-3-(phenylmethylene)- (9CI) (CA INDEX NAME)



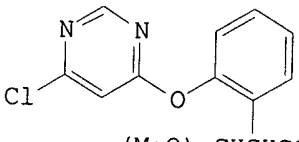
RN 147044-66-4 HCA
CN 5-Benzofurancarbonitrile, 7-chloro-2,3-dihydro-2-oxo-3-(phenylmethylene)- (9CI) (CA INDEX NAME)



L50 ANSWER 32 OF 162 HCA COPYRIGHT 2003 ACS
117:131219 a process for the preparation of 2-[(6-halo-4-pyrimidinyl)oxy]-.alpha.-(dimethoxymethyl)- and 2-[(6-halo-4-pyrimidinyl)oxy]-.alpha.-(methoxymethylene)benzeneacetates from 3-(methoxymethylene)- or 3-(dimethoxymethyl)-2(3H)-benzofuranone and dihalopyrimidine. Jones, John David; Deboos, Gareth Andrew; Wilkinson, Paul; Cox, Brian Geoffrey;

Fielden, Jan Michael (Imperial Chemical Industries PLC, UK). PCT Int. Appl. WO 9208703 A1 **19920529**, 49 pp. DESIGNATED STATES: W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MC, MG, MN, MW, NO, PL, RO, SD, SU, US; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1991-GB1989 19911112. PRIORITY: GB 1990-24992 19901116; GB 1990-24960 19901116; GB 1991-10592 19910516; GB 1991-12833 19910614; GB 1991-12832 19910614; GB 1991-13914 19910627; GB 1991-13911 19910627.

GI



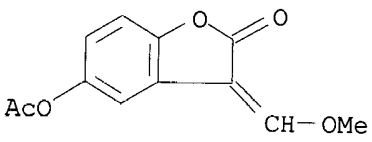
I

AB A process for the prepn. of 2-[(6-halo-4-pyrimidinyl)oxy]-.alpha.-(dimethoxymethyl)benzeneacetates and 2-[(6-halo-4-pyrimidinyl)oxy]-.alpha.-(methoxymethylene)benzeneacetates comprises the treatment of 3-(methoxymethylene)- or 3-(dimethoxymethyl)-2(3H)-benzofuranone with sodium methoxide followed by treatment with a 4,6-dihalopyrimidine. The phenoxypyrimidine derivs. thus prepd. are intermediates for fungicides (no data). A mixt. of 3-(methoxymethylene)-2(3H)-benzofuranone (8.8 g), THF (100 mL), and sodium methoxide (2.78 g) was added to 4,6-dichloropyrimidine (7.45 g) to give Me 2-[(6-chloro-4-pyrimidinyl)oxy]-.alpha.-(dimethoxymethyl)benzeneacetate (I). Salts of 3-(hydroxymethylene)-2(3H)-benzofuranone were prepd.

IT **143230-45-9P**, 5-Acetoxy-3-(methoxymethylene)-2(3H)-benzofuranone
143230-46-0P, 3-(Ethoxymethylene)-2(3H)-benzofuranone
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ring opening/condensation reaction of, with dihalopyrimidine)

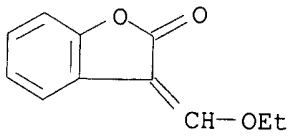
RN 143230-45-9 HCA

CN 2(3H)-Benzofuranone, 5-(acetyloxy)-3-(methoxymethylene)- (9CI) (CA INDEX NAME)



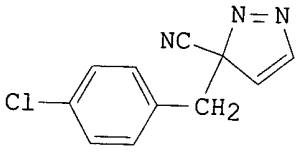
RN 143230-46-0 HCA

CN 2(3H)-Benzofuranone, 3-(ethoxymethylene)- (9CI) (CA INDEX NAME)



L50 ANSWER 37 OF 162 HCA COPYRIGHT 2003 ACS
115:114410 Effect of electron-withdrawing groups on the thermal ring opening of 3H-pyrazoles to diazoalkenes. Nakano, Yoshihiko; Hamaguchi, Masashi; Nagai, Toshikazu (Coll. Gen. Educ., Osaka Univ., Toyonaka, 560, Japan). Journal of Chemical Research, Synopses (7), 170-1 (English) **1991** . CODEN: JRPSDC. ISSN: 0308-2342.

GI



I

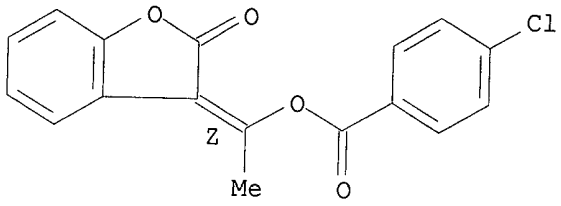
AB 3-Cyano-3H-pyrazoles, bearing a cyano, a p-chlorophenyl, or a p-chlorobenzyl group at C-3, e.g. I, generated from elimination reaction of the corresponding dihydropyrazoles with a leaving group such as a chlorine or p-chlorobenzoyloxy group, gave diazoalkene derivs., resulting from the ring-opening of the 3H-pyrazoles. 3-Methoxycarbonyl-3H-pyrazoles bearing a methoxycarbonyl, a p-chlorophenyl, or p-chlorobenzyl group at C-3, prepd. in a similar manner, gave mainly 1-methoxycarbonyl-1H-pyrazole derivs., resulting from migration of the 3-methoxycarbonyl group to the adjacent nitrogen within the generated 3H-pyrazoles. Treatment of 3H-pyrazoles and 5-substituted 1-methoxycarbonyl-1H-pyrazoles with triethylamine gave 3-substituted 1-methoxycarbonyl-1H-pyrazoles, resulting from migration of the methoxycarbonyl group to the remote nitrogen.

IT **135641-96-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 135641-96-2 HCA

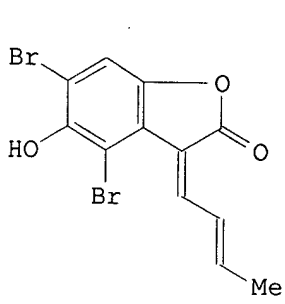
CN Benzoic acid, 4-chloro-, 1-(2-oxo-3(2H)-benzofuranylidene)ethyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

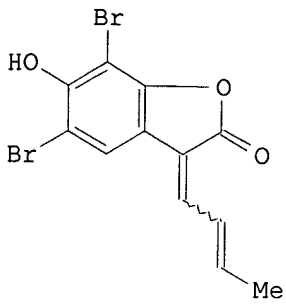


L50 ANSWER 45 OF 162 HCA COPYRIGHT 2003 ACS
110:212461 Aplysinadiene and (R,R)-5-[[3,5-dibromo-4-[(2-oxo-5-oxazolidinyl)]methoxy]phenyl]-2-oxazolidinone, two novel metabolites from Aplysina aerophoba. Synthesis of aplysinadiene. Norte, M.; Rodriguez, M. L.; Fernandez, J. J.; Eguren, L.; Estrada, D. M. (Inst. Univ. Quim. Org., Univ. La Laguna, La Laguna, 38206, Spain). Tetrahedron, 44(15), 4973-80 (English) **1988**. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 110:212461.

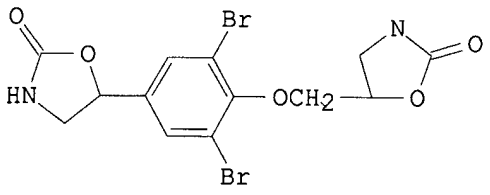
GI



I



II



III

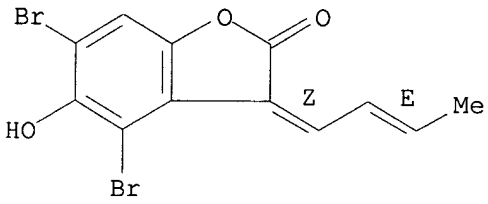
AB Two novel constituents, biogeneitcally derived from dibromotyrosine, were obtained from a sponge Aplysina aerophoba. The structure of aplysinadiene (I) was established on the basis of its spectral properties and by synthesis of I and its isomers (1'E)- and (1'Z)-II. The structure and abs. configuration of the oxazolidinone III was established by x-ray diffraction anal.

IT **108940-55-2P**, Aplysinadiene
RL: PREP (Preparation)
(isolation and mol. structure of)

RN 108940-55-2 HCA

CN 2(3H)-Benzofuranone, 4,6-dibromo-3-(2E)-2-butenylidene-5-hydroxy-, (3Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

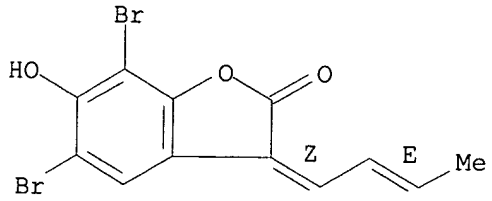


IT **108940-92-7P 108940-93-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 108940-92-7 HCA

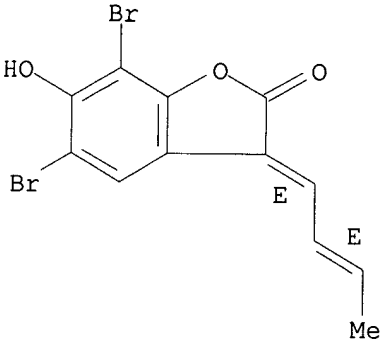
CN 2(3H)-Benzofuranone, 5,7-dibromo-3-(2-butenylidene)-6-hydroxy-, (Z,E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



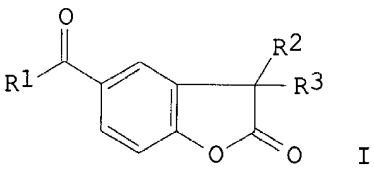
RN 108940-93-8 HCA
CN 2(3H)-Benzofuranone, 5,7-dibromo-3-(2-butenylidene)-6-hydroxy-, (E,E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L50 ANSWER 51 OF 162 HCA COPYRIGHT 2003 ACS
107:175814 5-Acyl-3-substituted benzofuran-2(3H)-ones as potential antiinflammatory agents. Chakrabarti, Jiban K.; Eggleton, Richard J.; Gallagher, Peter T.; Harvey, Janette; Hicks, Terence A.; Kitchen, E. Ann; Smith, Colin W. (Lilly Res. Cent. Ltd., Eli Lilly and Co., Windlesham /Surrey, GU20 6PH, UK). Journal of Medicinal Chemistry, 30(9), 1663-8 (English) **1987**. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 107:175814.

GI



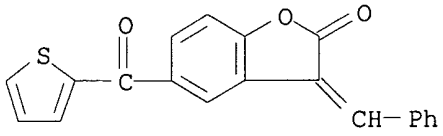
I

AB A series of substituted benzofuranones I (R1 = 2-thienyl, 2-furanyl, Ph; R2 = H, Me, Et, Pr; R3 = H, Me, Et; or R2R3 = PhCH) and their resp. ring-opened o-hydroxy acids were prepd. The antiinflammatory activity was evaluated in terms of their ability to improve adjuvant induced arthritis in rats. Their effect on the prodn. of both cyclooxygenase (CO) and lipoxygenase (LO) metabolites of arachidonic acid in guinea pig peritoneal polymorphonuclear neutrophils (PMNs) was also examd. No correlation between the antiinflammatory activity and increasing stability of the lactones could be found. The degree of activity in general shown by the

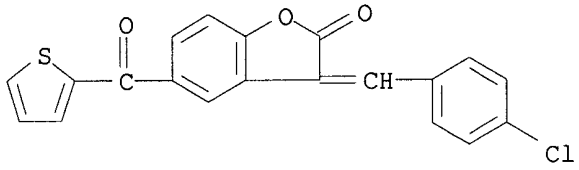
benzofuranones was similar to that of their corresponding o-hydroxy acids. This, coupled with the evidence from studies on opening of the lactone ring, suggests an in vivo transformation of the former into the latter. Benzofuranones displayed a dual inhibition of CO and LO products, while a moderate redn. in CO metabolites was shown by their acids.

IT **109217-49-4P 109217-50-7P 109217-51-8P**
109217-52-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antiinflammatory activity of)

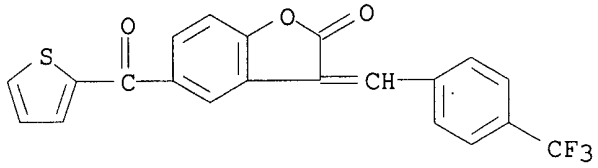
RN 109217-49-4 HCA
CN 2(3H)-Benzofuranone, 3-(phenylmethylene)-5-(2-thienylcarbonyl)- (9CI) (CA INDEX NAME)



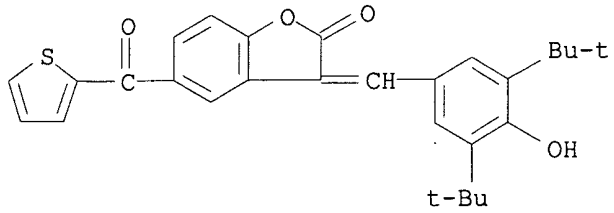
RN 109217-50-7 HCA
CN 2(3H)-Benzofuranone, 3-[(4-chlorophenyl)methylene]-5-(2-thienylcarbonyl)- (9CI) (CA INDEX NAME)



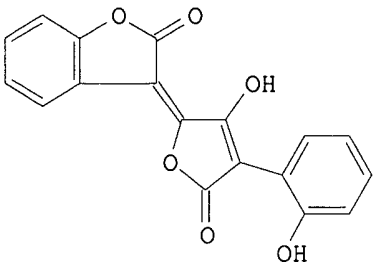
RN 109217-51-8 HCA
CN 2(3H)-Benzofuranone, 5-(2-thienylcarbonyl)-3-[[4-(trifluoromethyl)phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 109217-52-9 HCA
CN 2(3H)-Benzofuranone, 3-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]-5-(2-thienylcarbonyl)- (9CI) (CA INDEX NAME)



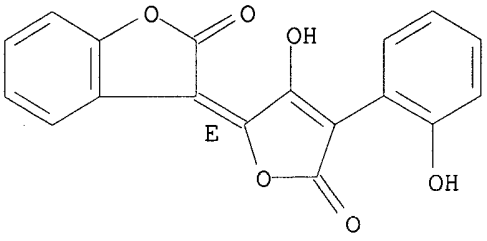
L50 ANSWER 58 OF 162 HCA COPYRIGHT 2003 ACS
103:6121 Synthesis of 2,2'-dimethoxypulvic acid and enolic structure of its demethylation product, 2-hydroxycalycin. Kuehler, Thomas C.; Nilsson, Martin; Sandberg, Ulla; Wachtmeister, Carl Axel (Dep. Org. Chem., Chalmers Univ., Goteborg, S-412 96, Swed.). Finnish Chemical Letters (4-5), 112-15 (English) **1984**. CODEN: FCMLAS. ISSN: 0303-4100.
GI



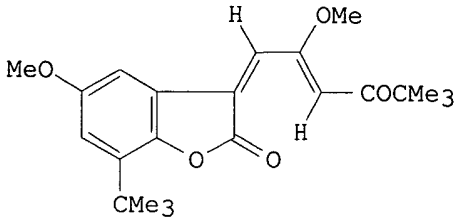
I

AB 2-Hydroxycalycin (I), an analog to the lichen compd. calycin, was synthesized via 2,5-bis(2-methoxyphenyl)-3,4-dioxoadiponitrile. Its structure was verified mainly by 1H-NMR spectrometry, which shows the presence of only one strong intramol. hydrogen bond.
IT **96700-90-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 96700-90-2 HCA
CN 2(3H)-Benzofuranone, 3-[3-hydroxy-4-(2-hydroxyphenyl)-5-oxo-2(5H)-furanylidene]-, (E)- (9CI) (CA INDEX NAME)

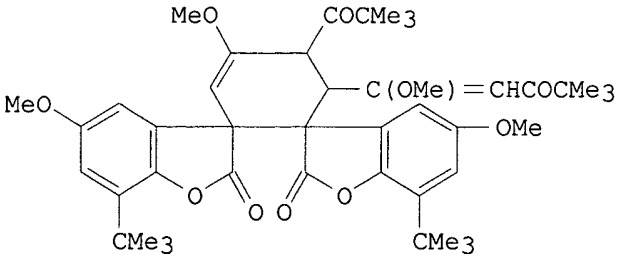
Double bond geometry as shown.



L50 ANSWER 63 OF 162 HCA COPYRIGHT 2003 ACS
99:22288 Diels-Alder dimerization of a hexenylidene-substituted benzofuran-2(3H)-one. Becker, Hans Dieter; Hall, Sydney R.; Skelton, Brian W.; White, Allan H. (Dep. Org. Chem., Chalmers Univ. Technol., Goeteborg, S-412 96, Swed.). Australian Journal of Chemistry, 36(2), 389-95 (English) **1983**. CODEN: AJCHAS. ISSN: 0004-9425.
GI



I



II

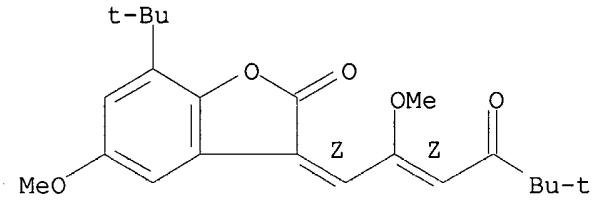
AB Benzofuranone I undergoes Diels-Alder dimerization in which the exocyclic double bond adds to the diene moiety. The stereochem. of the Diels-Alder dimer II was established by crystal x-ray structure detn. In II two benzofuranone moieties are situated so as to be vicinal spiro substituents of the cyclohexene formed in the Diels-Alder addn. The bond between the two benzofuranone units is unusually long. The shielding of one arom. hydrogen in the NMR spectrum of the dimer results from the disposition of the two arom. systems.

IT **64309-44-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(Diels-Alder dimerization of)

RN 64309-44-0 HCA

CN 2(3H)-Benzofuranone, 7-(1,1-dimethylethyl)-5-methoxy-3-(2-methoxy-5,5-dimethyl-4-oxo-2-hexenylidene)-, (Z,Z)- (9CI) (CA INDEX NAME)

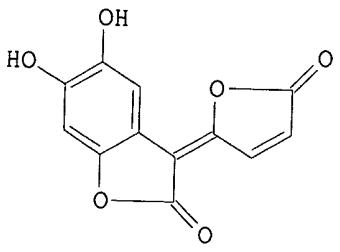
Double bond geometry as shown.



L50 ANSWER 69 OF 162 HCA COPYRIGHT 2003 ACS

95:76888 Fungal pigments. 38. Metabolites of 1,2,4-trihydroxybenzene from fruiting bodies of Gomphidius maculatus and G. glutinosus (Boletales). Jaegers, Erhard; Steffan, Bert; Von Ardenne, Renata; Steglich, Wolfgang (Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300, Fed. Rep. Ger.). Zeitschrift fuer Naturforschung, C: Journal of Biosciences, 36C(5-6), 488-9 (German) **1981**. CODEN: ZNCBDA. ISSN: 0341-0382.

GI



I

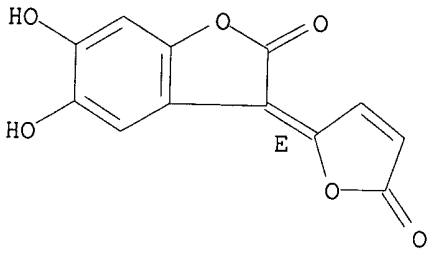
AB From fruiting bodies of Gomphidus 2,2',4,4',5,5'-hexahydroxybiphenyl and a red pigment, gomphilactone (I), were isolated. The latter may be derived biogenically from 1,2,4-trihydroxybenzene via oxidative dimerization to 3,5'-dihydroxydibenzoquinone followed by Posternak rearrangement.

IT **78570-66-8**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Gomphidius)

RN 78570-66-8 HCA

CN 2(3H)-Benzofuranone, 5,6-dihydroxy-3-(5-oxo-2(5H)-furanylidene)-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

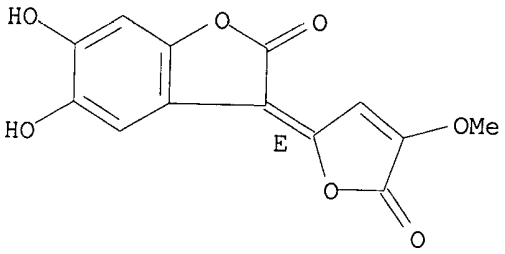


IT **78570-67-9P 78570-68-0P 78570-69-1P 78591-35-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 78570-67-9 HCA

CN 2(3H)-Benzofuranone, 5,6-dihydroxy-3-(4-methoxy-5-oxo-2(5H)-furanylidene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

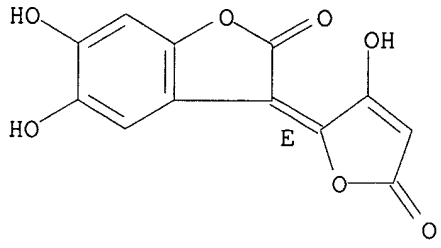


RN 78570-68-0 HCA

CN 2(3H)-Benzofuranone, 5,6-dihydroxy-3-(3-hydroxy-5-oxo-2(5H)-furanylidene)-

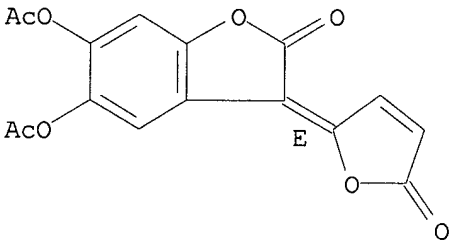
, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



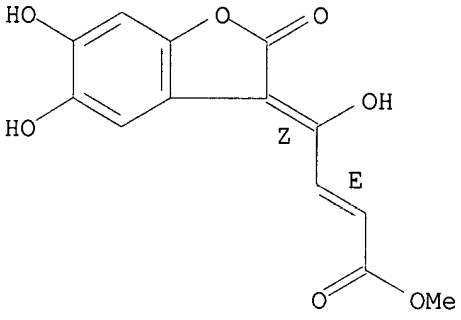
RN 78570-69-1 HCA
CN 2(3H)-Benzofuranone, 5,6-bis(acetyloxy)-3-(5-oxo-2(5H)-furanylidene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

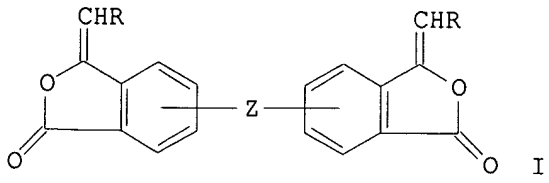


RN 78591-35-2 HCA
CN 2-Butenoic acid, 4-(5,6-dihydroxy-2-oxo-3(2H)-benzofuranylidene)-4-hydroxy-, methyl ester, (Z,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L50 ANSWER 70 OF 162 HCA COPYRIGHT 2003 ACS
95:62975 Polybenzopyrrolones. (Dainichiseika Color and Chemicals Mfg. Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 56041225 **19810417** Showa, 4 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1979-116121 19790912.
GI



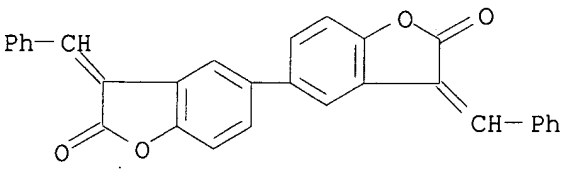
I

AB Sol., heat-resistant polybenzopyrrolones (d.p. 3-200) are manufd. by polymn. of bisbenzofuranone derivs. (I, Z is a bond or divalent moiety, R = Ph or substituted Ph), such as 5,5-bis(3-benzylidene-3H-benzofuran-2-one) [prepd. from 5,5'-bis(3H-benzofuran-2,7-dione [2420-87-3] and PhOAc [122-79-2]] with diamines such as 4,4'-diaminodiphenylmethane in inorg. solvent such as N-methyl-2-pyrrolidone at 200-80.degree. for 1-100 h.

IT **78544-63-5DP**, polymers with diamines
RL: IMF (Industrial manufacture); PREP (Preparation)
(heat-resistant, manuf. of)

RN 78544-63-5 HCA

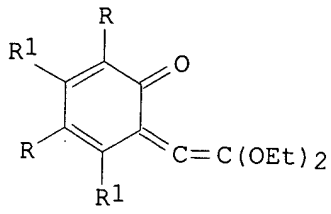
CN [5,5'-Bibenzofuran]-2,2'(3H,3'H)-dione, 3,3'-bis(phenylmethylene)- (9CI) (CA INDEX NAME)



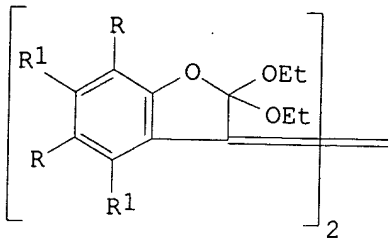
L50 ANSWER 72 OF 162 HCA COPYRIGHT 2003 ACS

94:14950 Push-pull-substituted allenes. IV. Synthesis and properties of 0-quinoid donor/acceptor-substituted allenes. Crystal and molecular structure of E-2,2,2',2'-tetraethoxy-.DELTA.3,3'(2H,2'H)-bi(phenanthro[9,10-b]furan). Saalfrank, Rolf W.; Ackermann, Erich; Winkler, Herbert; Paul, Winfried; Boehme, Reinhild (Inst. Org. Chem., Univ. Erlangen-Nuernberg, Erlangen, D-8520, Fed. Rep. Ger.). Chemische Berichte, 113(9), 2950-8 (German) **1980**. CODEN: CHBEAM. ISSN: 0009-2940.

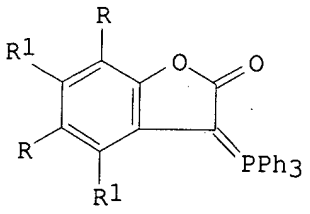
GI



I



III



V

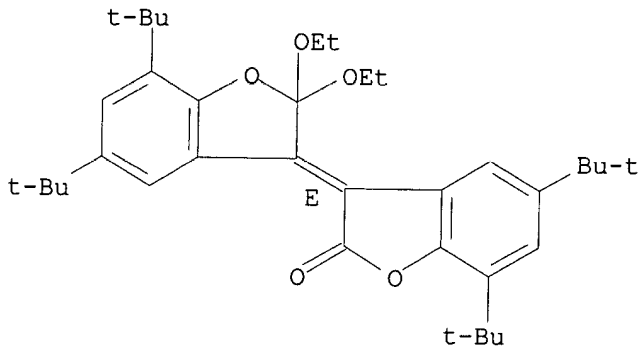
AB Reaction of Ph3P:C:C(OEt)2 with 3,5-di-tert-butyl-o-benzoquinone or 9,10-phenanthrenequinone yielded the donor/acceptor allene intermediates I (R = Me3C, R1 = H or RR1 = benzo) via oxaphosphetanes. I gave carbenes (II), which spontaneously dimerized forming III. The temp. dependence of the 1H NMR spectra led to insights into the diastereoisomerization of torsionally distorted III (RR1 = benzo) (IV) and the conformational mobility of the E-isomer. Acidic hydrolysis of Z/E-III (R = Me3C, R1 = H) led to the mono- and dilactones. The monomers I/II can be trapped by Ph3P to afford V following ether elimination. The structure of (E)-IV was detd. from x-ray data.

IT **75540-63-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)

RN 75540-63-5 HCA

CN 2(3H)-Benzofuranone, 3-[5,7-bis(1,1-dimethylethyl)-2,2-diethoxy-3(2H)-benzofuranylidene]-5,7-bis(1,1-dimethylethyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

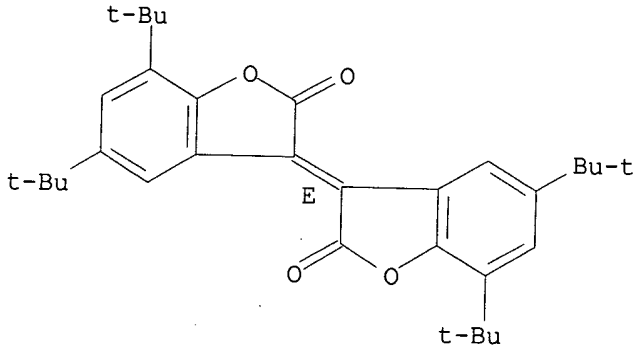


IT **75540-64-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 75540-64-6 HCA

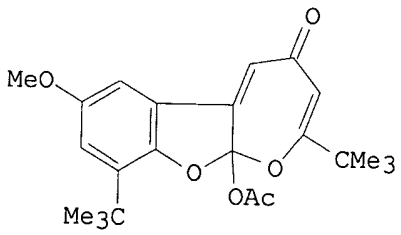
CN 2(3H)-Benzofuranone, 3-[5,7-bis(1,1-dimethylethyl)-2-oxo-3(2H)-benzofuranylidene]-5,7-bis(1,1-dimethylethyl)-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

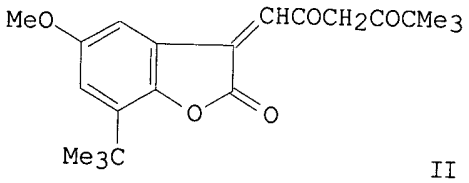


L50 ANSWER 76 OF 162 HCA COPYRIGHT 2003 ACS
91:91527 Oxidation of alkoxyphenols. Part 23. A re-examination of the reaction of 5,5'-dimethoxy-3,3'-di-tert-butylbiphenyl-2,2'-diol with lead tetraacetate: crystal structure of the product. Hewgill, F. Richmond; Hewitt, David G.; Howie, Graeme B.; Raston, Colin L.; Webb, Rauleigh J.; White, Allan H. (Sch. Chem., Univ. Western Australia, Nedlands, Australia). Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (2), 290-8 (English) **1979**. CODEN: JCPRB4. ISSN: 0300-922X.

GI



I



II

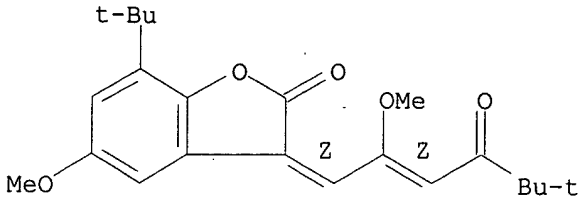
AB Pb(OAc)4 oxidn. of the title diol gave oxepinobenzofuran I, previously described as an acetoxybenzoxete (Hewgill, F. R.; Howie G. B., 1978), as a minor product. The structure of I is based on x-ray-crystallog. anal. of its benzoate. Redn. of I gave products contg. the biphenyl nucleus, whereas treatment with acid gave benzofuran-3(2H)-one derivs. E.g., with AcOH, I gave 59% benzofuranone II.

IT **64309-44-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)

RN 64309-44-0 HCA

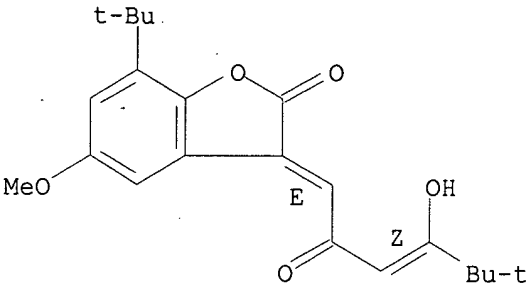
CN 2(3H)-Benzofuranone, 7-(1,1-dimethylethyl)-5-methoxy-3-(2-methoxy-5,5-dimethyl-4-oxo-2-hexenylidene)-, (Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



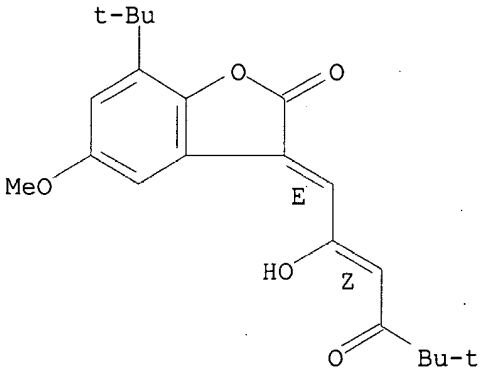
IT **71200-29-8P 71200-35-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 71200-29-8 HCA
CN 2(3H)-Benzofuranone, 7-(1,1-dimethylethyl)-3-(4-hydroxy-5,5-dimethyl-2-oxo-3-hexenylidene)-5-methoxy-, (Z,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



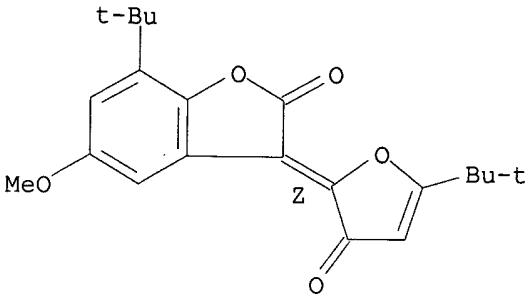
RN 71200-35-6 HCA
CN 2(3H)-Benzofuranone, 7-(1,1-dimethylethyl)-3-(2-hydroxy-5,5-dimethyl-4-oxo-2-hexenylidene)-5-methoxy-, (Z,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



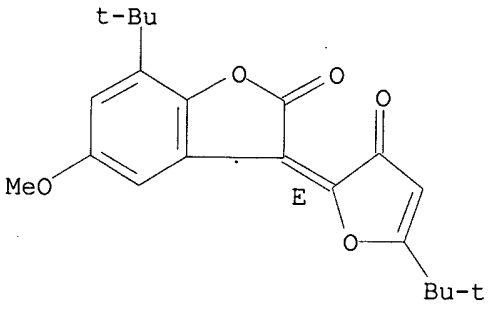
IT **71200-31-2P 71200-32-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 71200-31-2 HCA
CN 2(3H)-Benzofuranone, 7-(1,1-dimethylethyl)-3-[5-(1,1-dimethylethyl)-3-oxo-2(3H)-furanylidene]-5-methoxy-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

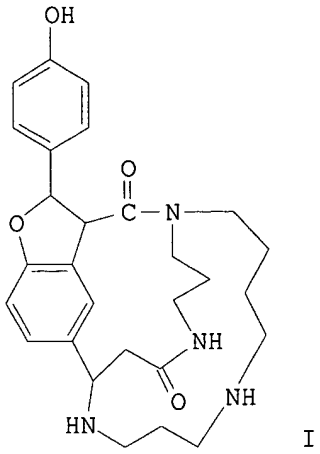


RN 71200-32-3 HCA
CN 2(3H)-Benzofuranone, 7-(1,1-dimethylethyl)-3-[5-(1,1-dimethylethyl)-3-oxo-2(3H)-furanylidene]-5-methoxy-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L50 ANSWER 78 OF 162 HCA COPYRIGHT 2003 ACS
90:138070 The structure of the spermine alkaloid aphelandrine from Aphelandra squarrosa Nees. Daetwyler, Peter; Bosshardt, Herbert; Bernhard, Heinz O.; Hesse, Manfred; Johne, Siegfried (Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.). Helvetica Chimica Acta, 61(7), 2646-71 (German) **1978**.
CODEN: HCACAV. ISSN: 0018-019X.
GI



I

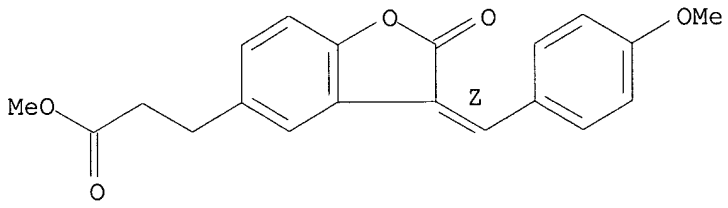
AB The structure of aphelandrine from A. squarrosa was detd. to be I from chem. and spectral data.

IT **69721-89-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dehydration of)

RN 69721-89-7 HCA

CN 5-Benzofuranpropanoic acid, 2,3-dihydro-3-[(4-methoxyphenyl)methylene]-2-oxo-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

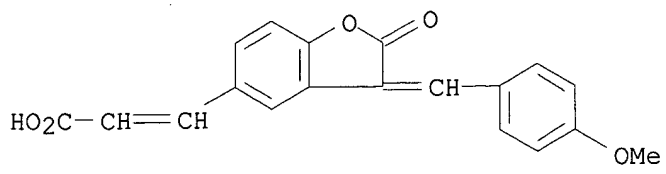
Double bond geometry as shown.



IT **69721-63-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)

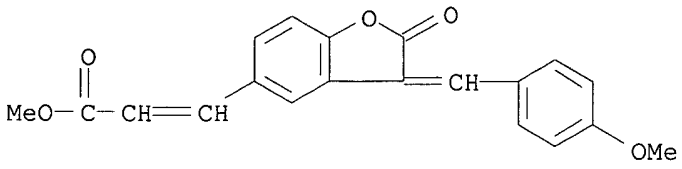
RN 69721-63-7 HCA

CN 2-Propenoic acid, 3-[2,3-dihydro-3-[(4-methoxyphenyl)methylene]-2-oxo-5-benzofuranyl]- (9CI) (CA INDEX NAME)



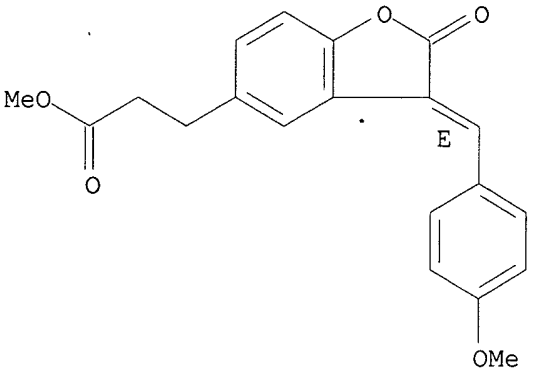
IT **69721-64-8P 69721-78-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 69721-64-8 HCA
CN 2-Propenoic acid, 3-[2,3-dihydro-3-[(4-methoxyphenyl)methylene]-2-oxo-5-benzofuranyl]-, methyl ester (9CI) (CA INDEX NAME)



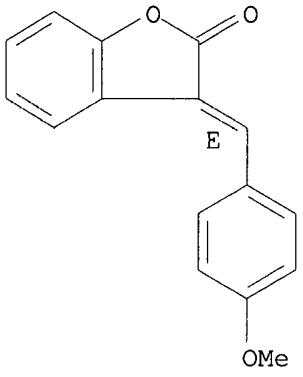
RN 69721-78-4 HCA
CN 5-Benzofuranpropanoic acid, 2,3-dihydro-3-[(4-methoxyphenyl)methylene]-2-oxo-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



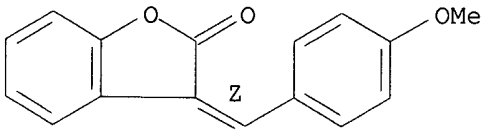
IT **59020-02-9 59020-03-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(spectral characteristics of)
RN 59020-02-9 HCA
CN 2(3H)-Benzofuranone, 3-[(4-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

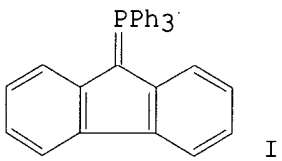


RN 59020-03-0 HCA
CN 2(3H)-Benzofuranone, 3-[(4-methoxyphenyl)methylene]-, (3Z)- (9CI) (CA INDEX NAME)

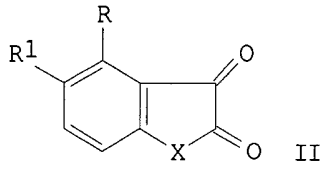
Double bond geometry as shown.



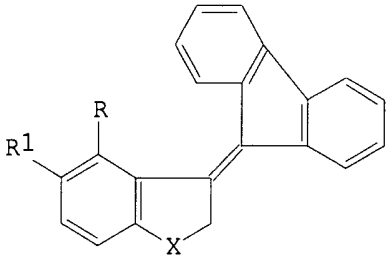
L50 ANSWER 80 OF 162 HCA COPYRIGHT 2003 ACS
89:129605 Organophosphorus compounds. XXVII. The reaction of fluorenylidenetriphenylphosphorane and triphenylphosphine with 2,3-benzofurandione, benzo[b]thiophene-2,3-dione, and naphtho[2,1-b]furan-1,2-dione. Sidky, M. M.; Boulos, L. S. (Natl. Res. Cent., Cairo, Egypt). Phosphorus and Sulfur and the Related Elements, 4(3), 299-302 (English) **1978**. CODEN: PREEDF. ISSN: 0308-664X.
GI



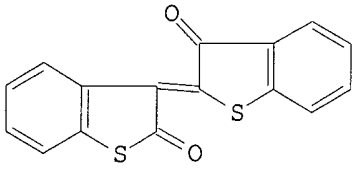
I



II



III



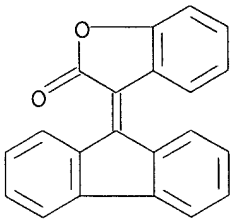
IV

AB Reaction of phosphorane I with diones II (R = R1 = H, X = O, S; RR1 = benzeno, X = O) gave 88, 85, 85% resp. III. Reaction of II (R = R1 = H, X = S) with Ph3P gave 92% IV. II (R = R1 = H, RR1 = benzeno, X = O) did not react with Ph3P.

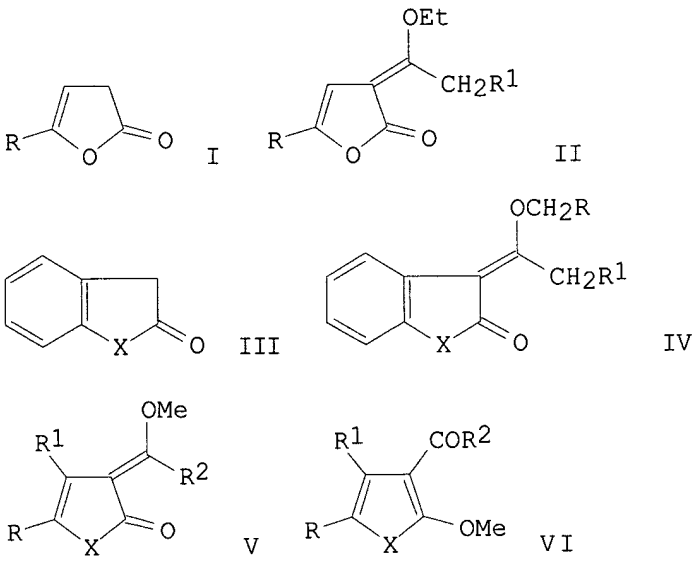
IT **67622-37-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 67622-37-1 HCA

CN 2(3H)-Benzofuranone, 3-(9H-fluoren-9-ylidene)- (9CI) (CA INDEX NAME)



L50 ANSWER 90 OF 162 HCA COPYRIGHT 2003 ACS
85:32744 Synthesis of .alpha.-alkoxyalkylidene-.DELTA..beta.,.gamma.-butenolides and analogous derivatives. Wolfers, Heinz; Kraatz, Udo; Korte, Friedhelm (Inst. Oekol. Chem., Tech. Univ. Muenchen, Munich, Fed. Rep. Ger.). Chemische Berichte, 109(3), 1061-8 (German) **1976**. CODEN: CHBEAM. ISSN: 0009-2940.
GI



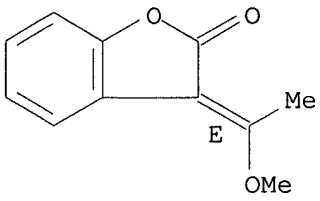
AB Et orthocarboxylates R1CH2C(OEt)3 (R1 = H, Me) condensed with butenolides I (R = Me, Et, Ph) to give 30-75% alkoxyalkylidene derivs. II (R = Me, Et, Ph; R1 = H; R = Et, R1 = Me; R = R1 = Me). R1CH2(OCH2R)3 (R = Me, R1 = H, Me, Ph; R = R1 = H) and the benzolog analogs III (X = O, S, NH, NMe) of I similarly gave 20-90% IV (12 compds.). Similar products (V, R = Ph, R1 = H, R2 = Me, Ph, X = O; RR1 = CH:CHCH:CH, R2 = Me, X = O, NMe; RR1 = CH:CHCH:CH, R2 = Ph, X = NMe) in addn. to ketones VI (R's and X as above) were formed when CH2N2 reacted with .alpha.-acyl-.DELTA..beta.,.gamma.-butenolides. Both methods give only (E)-alkoxyalkylidene derivs.

IT **32477-82-0P 59624-32-7P 59624-33-8P 59624-34-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 32477-82-0 HCA

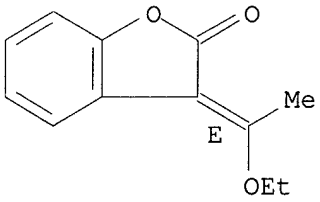
CN 2(3H)-Benzofuranone, 3-(1-methoxyethylidene)-, (E)- (8CI, 9CI) (CA INDEX NAME)

Double bond geometry as shown.



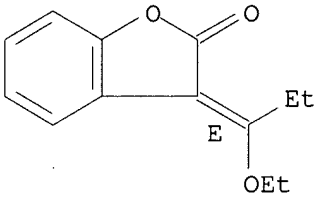
RN 59624-32-7 HCA
CN 2(3H)-Benzofuranone, 3-(1-ethoxyethylidene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



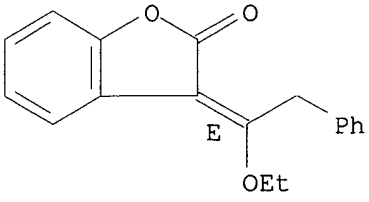
RN 59624-33-8 HCA
CN 2(3H)-Benzofuranone, 3-(1-ethoxypropylidene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 59624-34-9 HCA
CN 2(3H)-Benzofuranone, 3-(1-ethoxy-2-phenylethylidene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L50 ANSWER 100 OF 162 HCA COPYRIGHT 2003 ACS
81:3726 Heterocyclic semicarbazones and thiosemicarbazones. XXXI. Reaction

of coumarandione with aniline and hydrazines. Tomchin, A. B.; Ioffe, I. S.; Rusakov, E. A. (USSR). Zhurnal Organicheskoi Khimii, 10(3), 604-10 (Russian) **1974**. CODEN: ZORKAE. ISSN: 0514-7492.

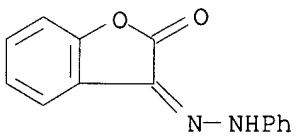
GI For diagram(s), see printed CA Issue.

AB The coumarandione I reacted with RNH2 (R = Ph, PhNH, NH2CSNH) in C6H6 to give 2-HOC6H4COCONHR (II); condensation of II (R = Ph) with H2NNHC(X)NH2 (X = S, O) gave 2-HOC6H4C [: NHNHC(X)NH2]CONHPh. I reacted with PhNH2 and H2NNHCONH2 in aq. alc. to give 2-HOC6H4C(:NPh)CO2H and 2-HOC6H4-C(:NNHCONH2)CO2H, resp. II (R = PhNH, H2NCONH) were refluxed in HOAc to give the corresponding coumarandione hydrazones III.

IT **17892-66-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 17892-66-9 HCA

CN 2,3-Benzofurandione, 3-(phenylhydrazone) (8CI, 9CI) (CA INDEX NAME)



L50 ANSWER 112 OF 162 HCA COPYRIGHT 2003 ACS

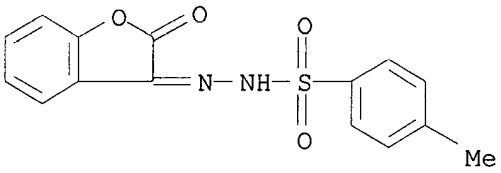
75:151615 Thermal and photoreactions of benzo- and naphthofurandiones (coumarandiones). Horspool, W. M.; Khandelwal, G. D. (Dep. Chem., Univ. Dundee, Dundee, UK). Journal of the Chemical Society [Section] C: Organic (20), 3328-31 (English) **1971**. CODEN: JSOOAX. ISSN: 0022-4952.

AB Thermal reaction of nucleophiles with 2,3-benzofurandione (I) gave ring cleavage to (o-hydroxyphenyl)glyoxylic acid derivs., e.g. PhNH2 gave the anilide and MeOH the Me ester. I and naphtho[2,1-b]furan-1,2-dione (II) with (p-tolylsulfonyl)hydrazine gave the 3- and 1-(p-tolylsulfonyl)hydrazones, resp., which were reduced to the corresponding diazo compds. I lost CO on irradn. to give salicylic acid derivs., probably via keto ketene intermediates, which could be trapped with acids to give anhydrides; II reacted similarly.

IT **34073-47-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 34073-47-7 HCA

CN p-Toluenesulfonic acid, (2-oxo-3(2H)-benzofuranylidene)hydrazide (8CI) (CA INDEX NAME)



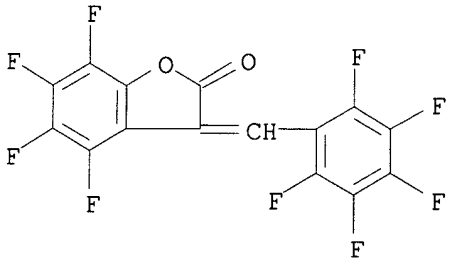
L50 ANSWER 120 OF 162 HCA COPYRIGHT 2003 ACS

71:124121 Transformations of decafluoro-.alpha.-phenylcinnamic acid. Molosnova, V. P.; Barkhash, V. A.; Vorozhtsov, N. N., Jr. (Novosibirsk. Inst. Org. Khim., Novosibirsk, USSR). Zhurnal Obshchei Khimii, 39(8), 1774-7 (Russian) **1969**. CODEN: ZOKHA4. ISSN: 0044-460X.

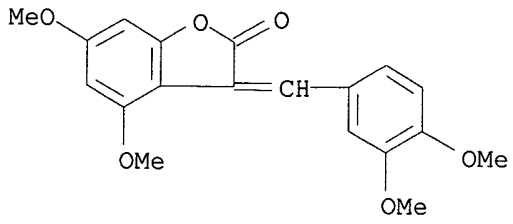
AB RMgCl from 20.8 g. C6F5Cl, prepd. in N atm. was treated with dry CH2O over

30-40 min., then treated with ice-HCl to yield 73% C6F5CH2OH, b57 113-14.5.degree., m. 30-1.degree.. C6F5CHO heated in Ac2O-Et3N with C6F5CH2CO2H (prepd. from above carbinol via treatment with PCl5, KCN and H2O), 0.5 hr. gave after acidification a mixt. of 63.6% C6F5CH:CPhCO2H (I), m. 187-8.degree., and 2% 3-pentafluorophenyl-5,6,7,8-tetrafluorocoumarin, m. 210-11.degree.. I gave the S-benzylthiuronium salt, m. 167-7.5.degree.. I heated with KF in Me2NCHO 5 hrs. gave 3-pentafluorobenzylidene-4,5,6,7-tetrafluoro-2-coumarone, m. 185-7.degree., which with KMnO4 was oxidized to tetrafluorosalicylic acid, m. 169-70.degree.. I and 20% oleum in CHCl3 at 40.degree., treated with NaN3, then quenched in ice, gave 73.5% decafluorodeoxybenzoin, m. 81-2.degree.. Ir spectra were reported.

IT **24043-88-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 24043-88-7 HCA
CN 2(3H)-Benzofuranone, 4,5,6,7-tetrafluoro-3-(2,3,4,5,6-pentafluorobenzylidene)- (8CI) (CA INDEX NAME)



L50 ANSWER 125 OF 162 HCA COPYRIGHT 2003 ACS
68:95457 Synthesis of .alpha.,2'-diacetoxy-3,4,4',6'-tetramethoxychalcone and 4,6,3',4'-tetramethoxyisoaurone. Clark-Lewis, John W.; Jemison, R. W. (Flinders Univ. South Australia, Bedford Park, Australia). Australian Journal of Chemistry, 21(3), 815-16 (English) **1968**. CODEN: AJCHAS. ISSN: 0004-9425.
GI For diagram(s), see printed CA Issue.
AB The synthesis of .alpha.,2'-diacetoxy-3,4,4',6'-tetramethoxychalcone (I) and 4,6,3',4'-tetramethoxyisoaurone (II) from the chalcone anion (III) is reported. Cyclization of 2'-hydroxy-2,3,4,4',6'-pentamethoxychalcone gave 2-hydroxy-4,6-dimethoxy-2-(3,4-dimethoxybenzyl)coumaran-3-one (IV), which in methanolic NaOH formed the Na salt of III. Treatment of the salt with Ac2O and NaOAc gave a mixt. of I and II which were sepd. by fractional crystn. II was formed by the benzilic acid rearrangement of III to the corresponding carboxylate anion and its structure was inferred from ir, N.M.R., and mass spectrometric data.
IT **18087-47-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 18087-47-3 HCA
CN 2(3H)-Benzofuranone, 4,6-dimethoxy-3-veratrylidene- (8CI) (CA INDEX NAME)



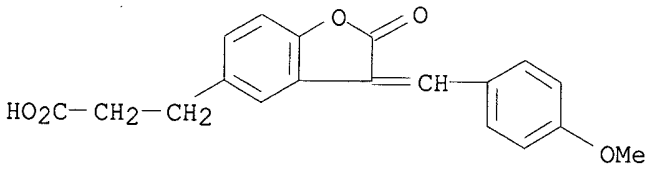
L50 ANSWER 130 OF 162 HCA COPYRIGHT 2003 ACS
67:73830 Antifungal factors in barley. IV. Isolation, structure, and synthesis of the hordatines. Stoessl, Albert (Canada Dep. Agr., London, UK). Canadian Journal of Chemistry, 45(15), 1745-60 (English) **1967**. CODEN: CJCHAG. ISSN: 0008-4042.

AB cf. CA 64: 6956a. Careful fractionation of exts. prepd. from barley coleoptiles gave small amts. of pure hordatines A and B and substantial amts. of a mixt. of their glucosides. The structures of the hordatines were deduced by degradative and spectroscopic studies and by the synthesis of some degradation products. A synthesis of racemic hordatine A analogous to its probable biogenesis was achieved by the oxidative coupling of coumaroylagmatine. The possible role of the hordatines in lignification is briefly discussed. 25 references.

IT **6522-00-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 6522-00-5 HCA

CN 5-Benzofuranpropionic acid, 2,3-dihydro-3-(p-methoxybenzylidene)-2-oxo- (8CI) (CA INDEX NAME)



L50 ANSWER 135 OF 162 HCA COPYRIGHT 2003 ACS
64:51892 Original Reference No. 64:9672d-h,9673a-c New synthesis of 2-hydroxy-2-benzyl-3-coumaranones. Chopin, Jean; Durual, Pierre; Chadenson, Michele (Fac. Sci., Lyon). Bulletin de la Societe Chimique de France (12), 3572-7 (French) **1965**. CODEN: BSCFAS. ISSN: 0037-8968.

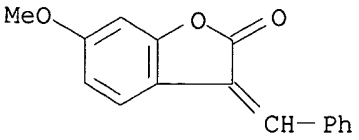
AB A series of 2-hydroxy-2-benzyl-3-coumaranones was prepd. by the debenzylation of the appropriate .alpha.-diketones obtained by the isomerization of 2'-benzyloxychalcones or of the corresponding 2'-benzyloxy-.alpha.-methoxychalcones. The existence of an equil. between the cyclic and open forms was demonstrated by their N. M.R. spectra and was in good agreement with the results of the alk. rearrangement of the 3-hydroxyflavanones. 2,4-(HO)2C6H3COCH2OMe (I) (5.5 g.) with Me2SO4 yielded 4.1 g. 2,4-HO(MeO)C6H3COCH2OMe (II), m. 65-6.degree. (EtOH). II (1.9 g.) with PhCH2Cl in HCONMe2 in the presence of NaI and K2CO3 gave 1.8 g. 2,4-phCH2O(MeO)C6H3COCH2OMe (III), m. 66.degree. (EtOH). I (2 g.) with PhCH2Cl gave similarly 2.6 g. 2,4-(PhCH2O)2C6H3COCH2OMe (IV), m. 104.degree. (EtOH). II (1 g.) and 1 g. BzH in 20 cc. EtOH treated overnight with 2 g. 50% ag. NaOH and acidified yielded 785 mg.

2,4-PhCH2O(MeO)C6H3COC(OMe):CHPh (V), m. 95.degree. (EtOH). V (1 g.) in 100 cc. MeOH and 20 cc. H2O refluxed 6 hrs. with 10 cc. concd. HCl gave 550 mg. yellow 2,4-PhCH2O(MeO)C6H3COCOCH2Ph, m. 86.degree. (EtOH). IV (1 g.) with 1 g. BzH gave 1.1 g. yellowish white 2,4-(PhCH2O)2-C6H3COC(OMe):CHPh (VI); m. 120.degree.. III (1 g.) and 1 g. p-MeOC6H4CHO yielded 815 mg. yellowish white 4-MeO analog of VI, m. 92-3.degree.. o-PhCH2OC6H4COCOCH2Ph (1 g.) in 20 cc. AcOH heated 1.5 hrs. on a water bath with 10 cc. concd. HCl yielded 585 mg. beige 2-hydroxy-2-benzyl-3-coumaranone (VII), m. 104.degree. (C6H6-hexane). o-PhCH2OC6H4COCH(OH)CHClPh gave similarly 78% VII. o-PhCH2OC6H4COCOCH2C6H4OMe-p (1 g.) gave similarly 490 mg. beige 4'-MeO deriv. (VIII) of VII, m. 120.degree. (C6H6-hexane). 3-Hydroxy-4'-methoxyflavanone (IX) (1 g.) heated 5 min. on the water bath with 100 cc. 2N alc. KOH and poured into 200 cc. 2N HCl gave 403 mg. 4'-methoxyflavonol (X), m. 228.degree. (EtOH); the filtrate from the X yielded 385 mg. oily o-HOC6H4C(OH)(CO2H)CH2C6H4OMe-p (XI) which gave an intense blue color with alc. FeCl3. The XI methylated with Me2SO4 and K2CO3 in MeOH gave o-MeOC6H4C(OH)(CO2Me)CH2C6H4OMe-p, m. 133.degree. (EtOH), which sapond. with alc. KOH yielded o-MeOC6H4C(OH)(CO2H)CH6C6H4OMe-p, m. 159.degree. (EtOH), and 190 mg. VIII, m. 120.degree.. VIII dehydrated with concd. H2SO4 gave 4'-methoxyaurone, m. 138-9.degree.. IX heated 15 min. on the water bath with alc. KOH gave 646 mg. XI and 296 mg. X. 4,2-MeO(PhCH2O)C6H3COCOCH2Ph (XII) (1 g.) with HCl-AcOH gave 435 mg. 6-MeO deriv. (XIII) of VII, m. 120.degree. (C6H6-hexane). XII (1 g.) in 20 cc. EtOH hydrogenated over 100 mg. 10% Pd-C, and the product chromatographed on Al2O3 yielded 450 mg. XIII. 4,2-MeO(PhCH2O)C6H3COCH(OH)CH-ClPh with HCl-AcOH gave 55% XIII. V gave similarly 57% XIII. XIII (100 mg.) and 2 cc. concd. H2SO4 heated 10 min. on the water bath gave 76 mg. 6-methoxyaurone, m. 145.degree. (EtOH). XIII (100 mg.) in 5 cc. EtOH and 3 cc. 2N KOH heated 3 min. on the water bath and acidified with 2N HCl yielded oily 2,4-HO(MeO)C6H3C(OH)(CO2H)CH2Ph (it gave an intense blue color with alc. FeCl3) which heated 3 min. on the water bath gave 79 mg. 6-methoxy-3-benzal-2-coumaranone, m. 129.degree. (MeOH). 4,-2-MeO(PhCH2O)C6H3COCOCH2C6H4OMe-p (1 g.) with HClAcOH yielded 470 mg. beige 4',6-dimethoxy deriv. (XIV) of VII, m. 111.degree. (C6H6-hexane). 4,2-MeO(PhCH2O)C6H3COC(OMe):CHC6H4OMe-p (500 mg.) gave similarly 225 mg. XIV. XIV treated with concd. H2SO4 gave 6,4'-dimethoxyaurone, m. 134.degree.. 2,4-(PhCH2O)2C6H3COC(OMe):CHPh (500 mg.) with HClAcOH gave 179 mg. 6-PhCH2 deriv. of VII, m. 186-7.degree. (C6H6), which dehydrated with concd. H2SO4 yielded 6-hydroxyaurone, m. 262-5.degree.. 2'-Hydroxy-3,4-dimethoxychalcone (8 g.) with Ac2O and AcONa gave 8 g. acetate, m. 90.degree., which treated in 100 cc. CS2 and 10 cc. CH2Cl2 with 1.25 cc. Br in 10 cc. CS2 and kept 1 hr. yielded 11 g. dibromide (XV), m. 162-3.degree. (CHCl3-hexane). XV (11 g.) refluxed 15 min. with 80 cc. Me2CO and 20 cc. H2O and heated 5 min. with 10 g. Na2CO3 in 70 cc. H2O gave 1.8 g. 3',4'-dimethoxyflavanol (XVI), m. 156-8.degree. (MeOH). 3-Hydroxy-3',4'-dimethoxyflavanone (XVII) heated 5 min. on the water bath with 2N alc. KOH gave 235 mg. 3-hydroxy-3',4'-dimethoxyflavone, m. 196-7.degree., 275 mg. o-HOC6H4C(OH)(CO2H)CH2C6H4(OMe)2-3,4 (XVIII) (it gave an intense blue color with alc. FeCl3), and 365 mg. 3',4'-dimethoxy deriv. of VII. XVIII with Me2SO4 yielded o-MeOC6H4C(OH)(CO2Me)CH2C6H3(OMe)2-3,4, m. 129.degree. (EtOH), which sapond. with alc. KOH gave o-MeOC6H4C(OH)(CO2H)CH2C6H3(OMe)2-3,4, m. 179.degree. (EtOH). XVII gave similarly during 15 min. 45% XVIII and 45% XVI.

IT **4940-53-8**, Acrylic acid, 2-(2-hydroxy-4-methoxyphenyl)-3-phenyl-, .gamma.-lactone
(prepn. of)

RN 4940-53-8 HCA

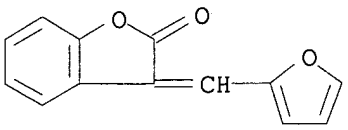
CN 2(3H)-Benzofuranone, 6-methoxy-3-(phenylmethylene)- (9CI) (CA INDEX NAME)



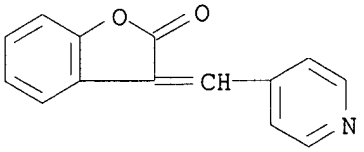
L50 ANSWER 140 OF 162 HCA COPYRIGHT 2003 ACS
62:9003 Original Reference No. 62:1618d-f Substituted .gamma.-lactones. XVI. Condensation of 2(3H)-benzofuranone with aromatic aldehydes. Walter, Roderich; Zimmer, Hans (Univ. of Cincinnati, Cincinnati, OH). Journal of Heterocyclic Chemistry, 1(4), 205-6 (English) **1964**. CODEN: JHTCAD. ISSN: 0022-152X.
GI For diagram(s), see printed CA Issue.
AB cf. CA 61, 14665b. A clear soln. of 0.01 mole 2(3H)-benzofuranone and 0.01 mole of an aromatic aldehyde treated with 2-10 drops of freshly distd. Et3N produced the corresponding analogs of I. The following I were reported (R, % yield, and m.p. given): 2-furyl, 56.5, 109.degree. (MeOH); 2-pyridyl, 69, 137.degree. (EtOH); 3-pyridyl, 34.5, 147.degree.; 4-pyridyl, 100, 148.degree.; 3,4-Cl2C6H3, 82.5, 188.degree.; 2,4-(O2N)2C6H3, 93, 206.degree. (HCONMe2); 2-BrC6H4, 79, 138.degree.; 4-BrC6H4, 99.6, 165.degree.; 2-ClC6H4, 99.5, 133.degree.; 3-ClC6H4, 78, 141.degree.; 4-ClC6H4, 94.5, 152.degree.; 2-FC6H4, 93, 124.degree.; 2-O2NC6H4, 75, 164.degree.; 3-O2NC6H4, 63.5, 194.degree.; 4-O2NC6H4, 94.5, 238.degree.; 4-MeC6H4, 51, 166.degree.; 3,4-(CH2O2)C6H3, 77.5, 205.degree.; 2-MeOC6H4, 89.5, 128.degree.; 3-MeOC6H4, 47.5, 101.degree.; 4-MeOC6H4, 83, 132.degree.; 2-O2NC6H4CH:CH, 99, 243.degree.; PhCH:CH, 92.5, 171.degree.; 2-EtOC6H4, 95, 96.degree.; 3,4-(MeO)2C6H3, 81.5, 99.degree.; 4-Me2NC6H4, 72, 208.degree.; 1-naphthyl, 66, 145.degree.; 2-naphthyl, 88, 126.degree.; 3,4-(EtO)2C6H3, 73, 129.degree..
IT **1019-20-1**, 2-Furanacrylic acid, .alpha.-(o-hydroxyphenyl)-, .gamma.-lactone **1022-38-4**, 4-Pyridineacrylic acid, .alpha.-(o-hydroxyphenyl)-, .gamma.-lactone **1022-39-5**, 2-Pyridineacrylic acid, .alpha.-(o-hydroxyphenyl)-, .gamma.-lactone **1025-44-1**, Acrylic acid, 3-(o-chlorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone **1025-45-2**, Acrylic acid, 3-(o-fluorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone **1025-47-4**, Acrylic acid, 3-(m-chlorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone **1025-48-5**, Acrylic acid, 2-(o-hydroxyphenyl)-3-p-tolyl-, .gamma.-lactone **1025-49-6**, Acrylic acid, 3-(p-chlorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone **1029-20-5**, Acrylic acid, 3-(3,4-dichlorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone **1029-21-6**, Acrylic acid, 2-(o-hydroxyphenyl)-3-(m-methoxyphenyl)-, .gamma.-lactone **1029-22-7**, Acrylic acid, 2-(o-hydroxyphenyl)-3-(p-methoxyphenyl)-, .gamma.-lactone **1029-25-0**, 2,4-Pentadienoic acid, 2-(o-hydroxyphenyl)-5-phenyl-, .gamma.-lactone **1032-73-1**, Acrylic acid, 2-(o-hydroxyphenyl)-3-(o-nitrophenyl)-, .gamma.-lactone **1032-74-2**, Acrylic acid, 2-(o-hydroxyphenyl)-3-(m-nitrophenyl)-, .gamma.-lactone **1032-75-3**, Acrylic acid, 2-(o-hydroxyphenyl)-3-(p-nitrophenyl)-, .gamma.-lactone **1032-99-1**, Acrylic acid, 2-(o-hydroxyphenyl)-3-[3,4-(methylenedioxy)phenyl]-, .gamma.-lactone **1090-41-1**, Acrylic acid, 3-[p-(dimethylamino)phenyl]-2-(o-hydroxyphenyl)-, .gamma.-lactone **1092-32-6**, Acrylic acid, 3-(3,4-dimethoxyphenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone **1092-33-7**, 2-Naphthaleneacrylic acid, .alpha.-(o-hydroxyphenyl)-, .gamma.-lactone **1092-44-0**, 1-Naphthaleneacrylic acid, .alpha.-(o-hydroxyphenyl)-, .gamma.-lactone **1097-12-7**, Acrylic acid, 3-(3,4-diethoxyphenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone

1147-87-1, Acrylic acid, 3-(o-bromophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone **1151-46-8**, Acrylic acid, 2-(o-hydroxyphenyl)-3-(o-methoxyphenyl)-, .gamma.-lactone **1160-29-8**, 2,4-Pentadienoic acid, 2-(o-hydroxyphenyl)-5-(o-nitrophenyl)-, .gamma.-lactone **1163-39-9**, Acrylic acid, 3-(2,4-dinitrophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone **1214-34-2**, 3-Pyridineacrylic acid, .alpha.-(o-hydroxyphenyl)-, .gamma.-lactone **1226-03-5**, Acrylic acid, 3-(o-ethoxyphenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone **4867-24-7**, Acrylic acid, 3-(p-bromophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone
(prepn. of)

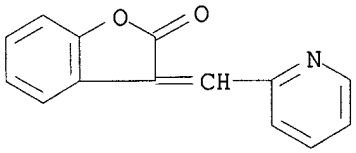
RN 1019-20-1 HCA
CN 2(3H)-Benzofuranone, 3-(2-furanylmethylene)- (9CI) (CA INDEX NAME)



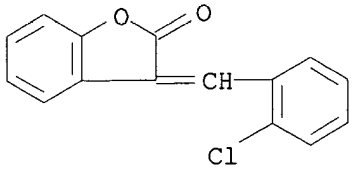
RN 1022-38-4 HCA
CN 2(3H)-Benzofuranone, 3-(4-pyridinylmethylene)- (9CI) (CA INDEX NAME)



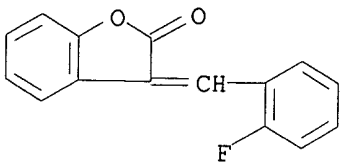
RN 1022-39-5 HCA
CN 2(3H)-Benzofuranone, 3-(2-pyridinylmethylene)- (9CI) (CA INDEX NAME)



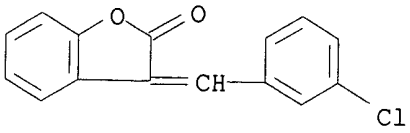
RN 1025-44-1 HCA
CN Acrylic acid, 3-(o-chlorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



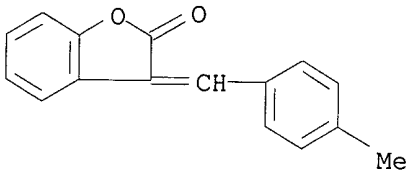
RN 1025-45-2 HCA
CN Acrylic acid, 3-(o-fluorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



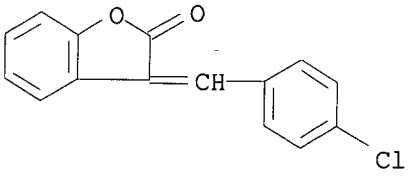
RN 1025-47-4 HCA
CN Acrylic acid, 3-(m-chlorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



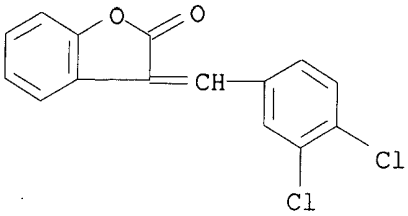
RN 1025-48-5 HCA
CN 2(3H)-Benzofuranone, 3-[(4-methylphenyl)methylene]- (9CI) (CA INDEX NAME)



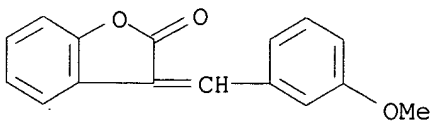
RN 1025-49-6 HCA
CN Acrylic acid, 3-(p-chlorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



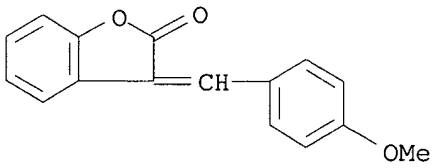
RN 1029-20-5 HCA
CN Acrylic acid, 3-(3,4-dichlorophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



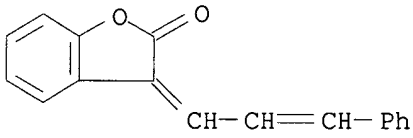
RN 1029-21-6 HCA
CN Acrylic acid, 2-(o-hydroxyphenyl)-3-(m-methoxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



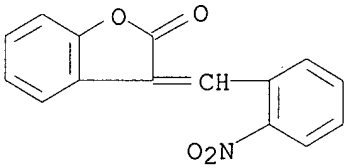
RN 1029-22-7 HCA
CN 2(3H)-Benzofuranone, 3-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



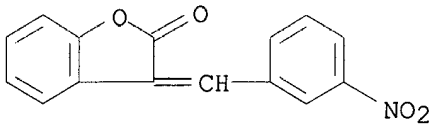
RN 1029-25-0 HCA
CN 2(3H)-Benzofuranone, 3-(3-phenyl-2-propenylidene)- (9CI) (CA INDEX NAME)



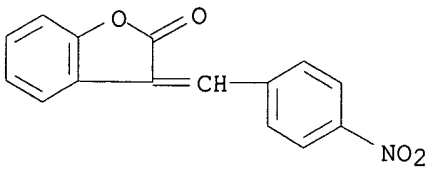
RN 1032-73-1 HCA
CN 2(3H)-Benzofuranone, 3-(o-nitrobenzylidene)- (8CI) (CA INDEX NAME)



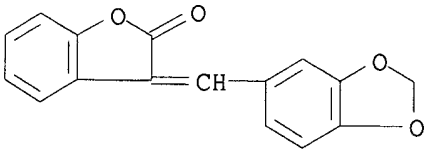
RN 1032-74-2 HCA
CN Acrylic acid, 2-(o-hydroxyphenyl)-3-(m-nitrophenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



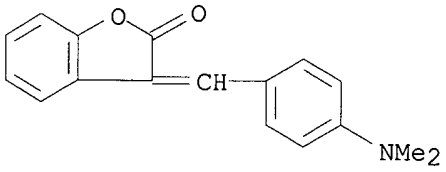
RN 1032-75-3 HCA
CN 2(3H)-Benzofuranone, 3-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)



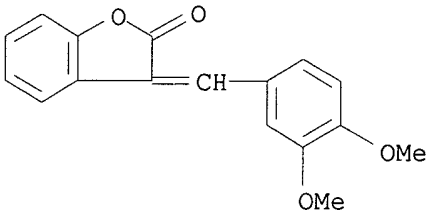
RN 1032-99-1 HCA
CN 2(3H)-Benzofuranone, 3-piperonylidene- (8CI) (CA INDEX NAME)



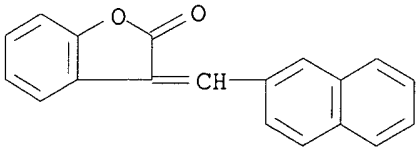
RN 1090-41-1 HCA
CN 2(3H)-Benzofuranone, 3-[[4-(dimethylamino)phenyl]methylene]- (9CI) (CA INDEX NAME)



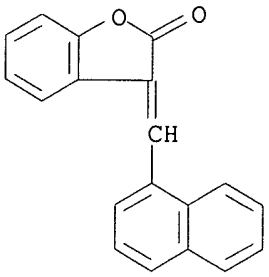
RN 1092-32-6 HCA
CN 2(3H)-Benzofuranone, 3-veratrylidene- (8CI) (CA INDEX NAME)



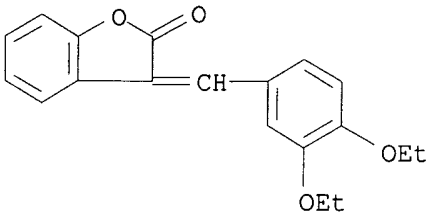
RN 1092-33-7 HCA
CN 2-Naphthaleneacrylic acid, .alpha.-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



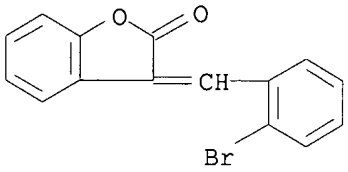
RN 1092-44-0 HCA
CN 1-Naphthaleneacrylic acid, .alpha.-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



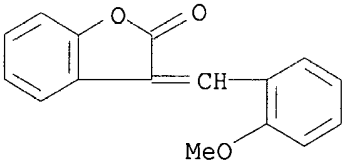
RN 1097-12-7 HCA
CN Acrylic acid, 3-(3,4-diethoxyphenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



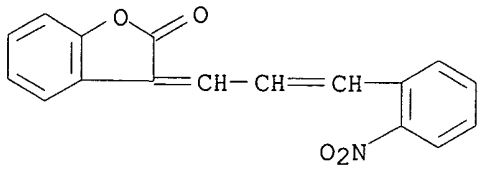
RN 1147-87-1 HCA
CN Acrylic acid, 3-(o-bromophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



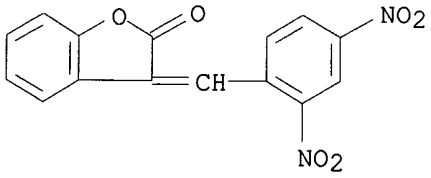
RN 1151-46-8 HCA
CN 2(3H)-Benzofuranone, 3-[(2-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



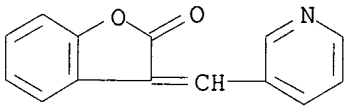
RN 1160-29-8 HCA
CN 2,4-Pentadienoic acid, 2-(o-hydroxyphenyl)-5-(o-nitrophenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



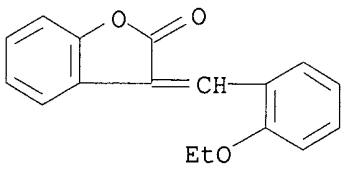
RN 1163-39-9 HCA
CN Acrylic acid, 3-(2,4-dinitrophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



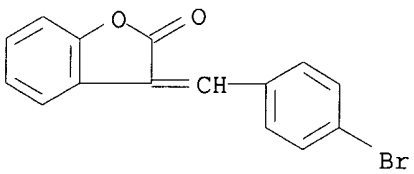
RN 1214-34-2 HCA
CN 3-Pyridineacrylic acid, .alpha.-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



RN 1226-03-5 HCA
CN Acrylic acid, 3-(o-ethoxyphenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



RN 4867-24-7 HCA
CN Acrylic acid, 3-(p-bromophenyl)-2-(o-hydroxyphenyl)-, .gamma.-lactone (7CI, 8CI) (CA INDEX NAME)



L50 ANSWER 145 OF 162 HCA COPYRIGHT 2003 ACS
57:36238 Original Reference No. 57:7214b-d A novel example of the alkaline rearrangement of 3-hydroxyflavanones. Chopin, Jean; Bouillant, Marie Louise (Fac. Sci., Lyons, Fr.). Compt. Rend., 254, 3699-701 (Unavailable)

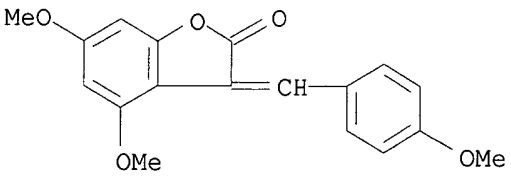
1962.

AB 4,5,7-Trimethoxyflavanol (I) (80 mg.) dissolved in 3 ml. EtOH, treated with 2 ml. 2N KOH, and heated 15 min. on a boiling water bath gave, after acidification and extn. with Et2O, 2 fractions. Fraction 1 was sol. in 5% NaOH, almost colorless, m. 120-5.degree., .lambda. 275 m.mu., gave a blue-green color with alc. FeCl3, and was probably 2,4,6-HO(MeO)2C6H2C(OH)(CO2H)CH2C6H4OMe-4 (II). On recrystn. of II from MeOH, 56% yellow crystals of 3-benzylidene-4,4',6trimethoxy-2-coumaranone (III) were obtained. Fraction 2 was 2-hydroxy-2-benzyl-4,4',6-trimethoxy-3-coumaranone (IV). Heating (I) 3 min. on the boiling water bath with 10% methanolic KOH gave only IV. IV heated 15 min. at 100.degree. with alc. KOH gave 12% III. In the series of flavanols derived from phloroglucinol, the behavior in alk. soln. of the 4'-methoxy deriv. was much closer to that of the 3',4',5' trimethoxy deriv. than to that of unsubstituted or 3',4'-dimethoxy derivs.

IT **64818-74-2**, Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(p-methoxyphenyl)-, .gamma.-lactone
(prepn. of)

RN 64818-74-2 HCA

CN 2(3H)-Benzofuranone, 4,6-dimethoxy-3-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



L50 ANSWER 150 OF 162 HCA COPYRIGHT 2003 ACS

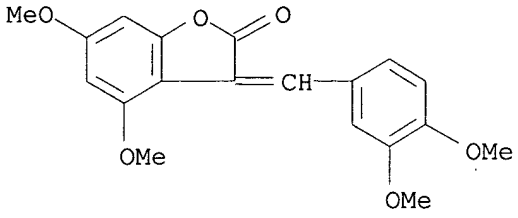
53:99778 Original Reference No. 53:17994i,17995a-c New synthesis of 3-benzalcoumarones. Molho, Darius Compt. rend., 248, 1535-7 (Unavailable) **1959.**

AB .alpha.-Methoxy-2'-hydroxy-4',6'dimethoxychalcones (I), 2-hydroxy-2-benzylcoumarones (II), or 2-methoxy-2-benzylcoumarones (III) (100 mg.) intimately mixed in a mortar with 700 mg. acid bentonite (dried in an oven at 300.degree. and kept in a stoppered flask), kept in a hemolysis tube 10-15 min. at 200-210.degree., cooled, the powder extd. several times with C6H6 or boiling Me2CO, the mixt. filtered, and the solvent evapd. give 3-benzalcoumarones (IV) or 2-benzalcoumarones (V) in 60-80% yields. I, prepd. by condensation of .omega.-methoxy-.omicron.-hydroxy-acetophenones with aromatic aldehydes, give III on heating without catalyst or in dil. alkali. Treated with alc. HCl, I undergo demethylation at the OMe .alpha. to the oxo group and cyclization to II. If acid bentonites are used instead of HCl, they play the role of Lewis acids, giving rise to a rearrangement, IV forming after dehydration. II, subjected to the same treatment, also give IV but III give V, without rearrangement. It is therefore assumed that on heating with bentonite demethylation occurs prior to any cyclization, and that the dioxo deriv. thus obtained is rearranged. The m.ps. are given for I, II, III, IV and V, resp., as a function of the substituents (the 3-, 4-, and 5-substituents on the benzyl group given): H, H, H, 112.degree., 172.degree., 108.degree., 176.degree., 153.degree.; OMe, OMe, OMe, 144.degree., 169.degree., 118.degree., 160.degree., 212.degree.; H, OMe, OMe, 117.degree., 176.degree., 117.degree., 173.degree., 173.degree.; H, OMe, H, 121.degree., 159.degree., 118.degree., 167.degree., 166.degree..

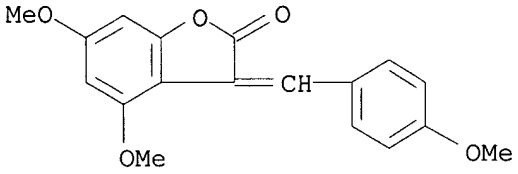
IT **18087-47-3**, Acrylic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4,6-dimethoxyphenyl)-, .gamma.-lactone **64818-74-2**, Acrylic acid,

2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(p-methoxyphenyl)-, .gamma.-lactone **102159-53-5**, Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)-, .gamma.-lactone **107153-09-3**, Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenyl-, .gamma.-lactone
(prepn. of)

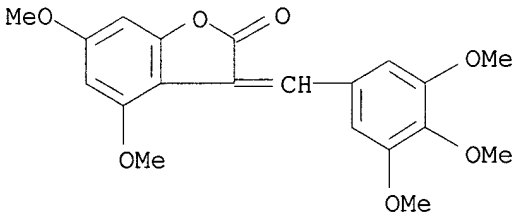
RN 18087-47-3 HCA
CN 2(3H)-Benzofuranone, 4,6-dimethoxy-3-veratrylidene- (8CI) (CA INDEX NAME)



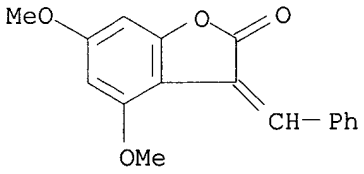
RN 64818-74-2 HCA
CN 2(3H)-Benzofuranone, 4,6-dimethoxy-3-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 102159-53-5 HCA
CN Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)-, .gamma.-lactone (6CI) (CA INDEX NAME)



RN 107153-09-3 HCA
CN Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenyl-, .gamma.-lactone (6CI) (CA INDEX NAME)



L50 ANSWER 155 OF 162 HCA COPYRIGHT 2003 ACS
51:43285 Original Reference No. 51:8063f-i,8064a-i,8065a-b Rearrangements of hydroxydiquinones. II. Rearrangement products of 2-hydroxy-4,4'-

ditoluquinone and of 2-hydroxy-4,4'-dimethoxydiquinone. Posternak, Th.; Huguenin, R.; Alcalay, W. (Univ. Lausanne, Switz.). Helv. Chim. Acta, 39, 1564-79 (French) **1956**.

GI For diagram(s), see printed CA Issue.

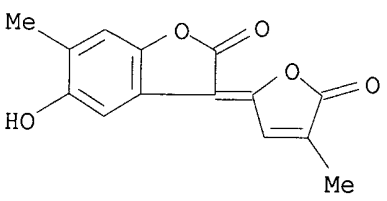
AB 2-Hydroxy-4,4'-ditoluquinone (I) (compd. VI of preceding part) (500 mg.) in 40 cc. hot MeOH treated with 20 cc. 10% H2SO4 and the mixt. refluxed 10 min. yielded 440 mg. 6,5-Me(RO)C6H2.O.CO.C:C.CH:CMe.CO.O (II, R = H) (IIa), m. 271-3.degree.. The rearrangement also took place in 70% AcOH at room temp., or in the same cold reagent starting with I, its acetate or its Me ether. IIa boiled 1-2 min. with 10 parts Ac2O contg. 1 part anhyd. NaOAc yielded II (R = Ac), m. 214-15.degree.. II (R = ClCH2CO) m. 249.degree.; II (R = o-ClC5H4CO) m. 233.degree.. IIa (1 g.) in 12 cc. hot N NaOH cooled, 3 cc. Me2SO4 and 16 cc. 2.4N NaOH added, the mixt. shaken 20 min., the reactions repeated 4 times, 16 cc. 2.4N NaOH added, and the product allowed to stand 4 hrs. and acidified to Congo red with concd. HCl yielded 0.74 g. II (R = Me) (III), m. 225-6.degree.. IIa (100 mg.) in 2 cc. AcOH heated to boiling, treated with 300 mg. Zn, filtered, and the filtrate poured into 10 parts cold water yielded 70 mg. butanolide analog (IV), m. 225-6.degree.. The butanolide analog (V) of III m. 174-5.degree.. IIa (1.2 g.) in 190 cc. hot AcOH cooled, treated with 4.65 cc. 6.07N CrO3 in AcOH, allowed to stand 30 min., the products of 4 reactions united, poured into 3 vols. water, extd. with CHCl3, the CHCl3 evapd., the residue digested with 10 cc. EtOH, the insol. part taken up in 300 cc. CHCl3, the soln. extd. 4 times with 100 cc. satd. Na-HCO3, then with M Na2CO3, the Na2CO3 soln. extd. with HCl, then with CHCl3, and the CHCl3 evapd. yielded 112 mg. (C8H6O3)n, m. 313-14.degree. (cor.). The bicarbonate exts. washed with CHCl3 and acidified yielded 1.58 g. OC.CH:CMe.CO.CH:CC(CO2H): C.CH:CMe.CO.O (VI), m. 239-40.degree. (cor., decompn.). VI heated under N lost CO2 and yielded a neutral product m. 254.degree.. VI titrated with iodine and the product decolorized with Na2S2O3 and extd. with CHCl3 yielded IIa. VI (46 mg.) treated at room temp. with 0.3 cc. 5% H2SO4 in Ac2O and the product allowed to stand 4 hrs. yielded 45 mg. VII, m. 240.degree.. III (544 mg.) in 45 cc. hot dioxane cooled, treated drop by drop with 20 cc. 6% KMnO4, filtered, the ppt. washed with aq. dioxane, the filtrates concd. in vacuo to 7-8 cc., the residue treated hot with 0.83 cc. 2.4N NaOH, these operations repeated 4 times, the alk. liquid concd. in vacuo to 1/3 vol., acidified to Congo red with 10N H2SO4, extd. 12 times with Et2O, the Et2O evapd., the residue in 10 cc. Me2CO treated drop by drop (ice cooling) with 1 cc. 6% KMnO4, filtered, the filtrate evapd. in vacuo, the residue in Et2O shaken with NaHCO3, and the ext. acidified and extd. with Et2O yielded 4,2,5-Me(MeO)2C6H2CO2H (VIII), m. 124-4.5.degree.. VI hydrazinolyzed yielded the hydrazide (IX), m. 197-8.degree., of 4,2,5-Me(HO)2C6H2CH2CO2H (IXa). The mother liquors yielded the dihydrazide (X) of mesaconic acid, m. 220.degree.. III with N2H4.H2O yielded the hydrazide (XI), m. 207-9.degree., of 4,2,5-Me(HO)-(MeO)C6H3CH2CO2H (XII); the mother liquors yielded X, m. 221.degree. (decompn.). IV (100 mg.) with N2H4.H2O yielded 50 mg. IX, m. 196-8.degree.; the gummy residue from the mother liquors boiled 3 hrs. with 4 cc. 0.5N Ba(OH)2 in MeOH, the Ba salt acidified exactly with H2SO4, the filtrate evapd., and the residue extd. with Et2O yielded dl-methylsuccinic acid, m. 110-12.degree.. XI (100 g.) heated 30 min. in a water bath with 2 cc. 2N NaOH, cooled, acidified to Congo red with HCl, and extd. with Et2O yielded 84 mg. XII, m. 121-3.degree.. 2,5-(MeO)2C6H3Me (31.5 g.), 120 cc. concd. HCl, and 53 cc. HCHO (38%) treated 2 hrs. with a stream of dry HCl (the temp. held at 95-100.degree. during the 2nd hr.), and the mixt. cooled and extd. with Et2O yielded 5-6 g. [4,3,6-Me(MeO)2C6H2]2CH2 (XIII), m. 144-6.degree.. The Et2O mother liquors yielded 17.3 g. 4,2,5-Me(MeO)2C6H2CH2Cl (XIV), b17 150-8.degree., m. 62-3.degree.. Molten XIV (13.2 g.) added to 40 g. NaCN, 65 cc. water, and 70 cc. EtOH, the mixt. refluxed 20 min., the EtOH distd., the residue

dild. with 1 vol. water, extd. with Et2O, and the ext. fractionated in vacuo yielded 1.30 g. 4,2,5-Me(MeO)2C6H2CH2CN (XV), m. 67-8.degree.; another fraction yielded 0.20 g. XV and a mixt. contg. 90% 4,2,5-EtO(MeO)2C6H3Me and 10% 4,2,5-Me(MeO)2C6H2CH2OH, which with dry HCl yielded XIV. XIV (1.15 g.) treated with NaCN and the residue sapond. with 6 cc. EtOH and 3.8 cc. water contg. 1.5 g. KOH yielded 700 mg. 4,2,5-Me(MeO)2C6H2CO2H (XVa), m. 131-2.degree., also obtained by methylation of 4,2,5-Me(MeO)C6H2CO2H (XVb). The hydrazide (1.78 g.) of XVa refluxed 7 hrs. with 50 parts 4N HCl, the HCl removed in vacuo, and the residue digested with 6 and 3 cc., resp., of water yielded IXa, m. 157.degree. (decompn.). IXa (220 mg.) distd. at 130-80.degree./0.1 mm. yielded 194 mg. 5-hydroxy-6-methyl-2-coumaranone (XVI), m. 163-4.degree., XVa (740 mg.) refluxed 1 hr. with 16 cc. 47% HBr, the HBr removed in vacuo, and the residue dried in vacuo over KOH yielded a mixt. of IXa and XVI which on distn. gave XVI, m. 161-3.degree.. XVb (50 mg.) heated 45 min. at 170-80.degree. (oil bath) yielded 30 mg. 5-methoxy-6-methyl-2-coumaranone (XVII), m. 104-6.degree.. XVI (78 mg.), 0.16 g. citraconic anhydride, and 0.02 cc. pyridine heated 4 min. at 155-60.degree. (the pyridine can be replaced by 5-6 mg. anhyd. NaOAc) and the cold mixt. dissolved in 2.5 cc. hot 2.3N NaOH and acidified with HCl yielded 70 mg. II, m. 272-3.degree.. XVI (69 mg.), 82 g. citraconic anhydride, and 7 mg. anhyd. NaOAc heated 10 min. at 155-60.degree. (oil bath), the cooled product treated with boiling water, and the residue recrystd. from AcOH yielded 44 mg. III, m. 226-7.degree.. 2,3,3',6,6'-Pentahydroxy-4,4'-dimethoxybiphenyl (3.1 g.) in 100 cc. boiling AcOH treated with 20 cc. water and 14.7 cc. 2.9N FeCl3 yielded 2.0 g. 6,5-MeO(R'O)C6H2.O.CO.C:C.CH:C(OMe).CO.O (XVIII, R' = H) (XVIIIa), m. 275-7.degree.; XVIII (R = Me) (XIX), m. 238-9.degree.; XVIII (R = Ac), m. 260-1.degree.. XVIIIa (333 mg.) in 1 cc. 99% N2H4.H2O allowed to stand overnight, the product evapd. to dryness in vacuo, and the residue treated with 0.8 cc. water yielded 95 mg. hydrazide, m. 198-200.degree. (decompn.), of 4,2,5-MeO(HO)2C6H2CH2CO2H; the aq. ext. contained CH2.CO.NH.N:CCONHNH2 (XX). XIX (200 mg.) treated 5 hrs. with 0.6 cc. N2H4.H2O yielded 55 mg. hydrazide, m. 177-8.degree., of 2,4,5-HO(MeO)2C6H4CH2CO2H; the mother liquors evapd. to dryness in vacuo, the residue treated with 0.5 cc. water and 0.5 cc. N AcOH yielded XX, m. 260.degree..

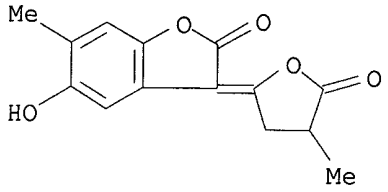
IT **80651-86-1**, Muconic acid, 2-(2,5-dihydroxy-p-tolyl)-3-hydroxy-5-methyl-, di-.gamma.-lactone **108487-90-7**, .alpha.-Hydromuconic acid, 2-(2,5-dihydroxy-p-tolyl)-3-hydroxy-5-methyl-, di-.gamma.-lactone **108900-07-8**, Muconic acid, 2-(2,5-dihydroxy-4-methoxyphenyl)-3-hydroxy-5-methoxy-, di-.gamma.-lactone **109342-75-8**, Muconic acid, 3-hydroxy-2-(2-hydroxy-5-methoxy-p-tolyl)-5-methyl-, di-.gamma.-lactone **109342-80-5**, Muconic acid, 3-hydroxy-2-(2-hydroxy-4,5-dimethoxyphenyl)-5-methoxy-, di-.gamma.-lactone **109442-63-9**, .alpha.-Hydromuconic acid, 3-hydroxy-2-(2-hydroxy-5-methoxy-p-tolyl)-5-methyl-, di-.gamma.-lactone
(prepn. of)

RN 80651-86-1 HCA

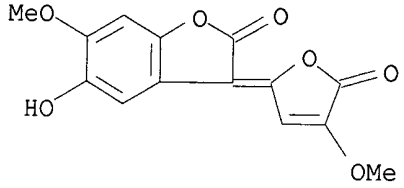
CN 2(3H)-Benzofuranone, 5-hydroxy-6-methyl-3-(4-methyl-5-oxo-2(5H)-furanylidene)- (9CI) (CA INDEX NAME)



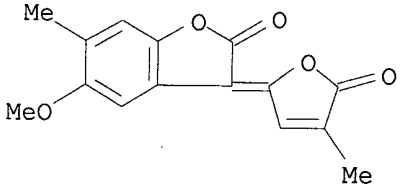
RN 108487-90-7 HCA
CN .alpha.-Hydromuconic acid, 2-(2,5-dihydroxy-p-tolyl)-3-hydroxy-5-methyl-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



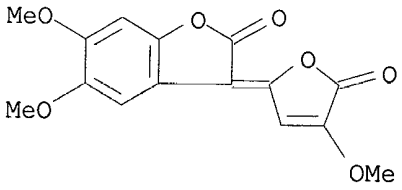
RN 108900-07-8 HCA
CN Muconic acid, 2-(2,5-dihydroxy-4-methoxyphenyl)-3-hydroxy-5-methoxy-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



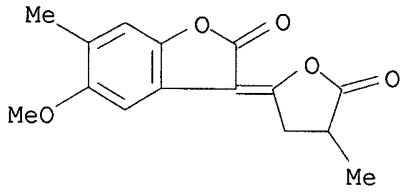
RN 109342-75-8 HCA
CN Muconic acid, 3-hydroxy-2-(2-hydroxy-5-methoxy-p-tolyl)-5-methyl-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



RN 109342-80-5 HCA
CN Muconic acid, 3-hydroxy-2-(2-hydroxy-4,5-dimethoxyphenyl)-5-methoxy-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



RN 109442-63-9 HCA
CN .alpha.-Hydromuconic acid, 3-hydroxy-2-(2-hydroxy-5-methoxy-p-tolyl)-5-methyl-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



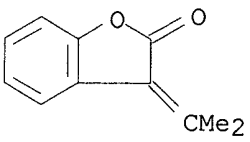
L50 ANSWER 160 OF 162 HCA COPYRIGHT 2003 ACS
50:1323 Original Reference No. 50:249b-d Claisen rearrangement of .gamma.-phenoxycrotonic acid esters. Canonica, Luigi; Fiecchi, Alberto (Univ. Milan). Atti accad. nazl. Lincei, Rend., Classe sci. fis., mat. e nat., 17, 385-90 (Unavailable) **1954**.

AB PhOCH2CH:CHCO2R (I) and PhOCH2CMe:CHCO2R (II) were studied under the conditions of the Claisen rearrangement. Besides a small portion which resinifies, I was recovered unaltered after 15 hrs. at 230.degree. or 270.degree. in an inert atm. This is an exception to the general reactivity of phenyl allyl ethers having a free ortho position (approx. 100 compds.) all of which rearrange at 180-220.degree. in 2-3 hrs. II (R = Me and Et) heated at 220.degree., however, rearrange, but the expected 2-(o-hydroxyphenyl)-3-methyl-3-butenoic esters were not obtained. Both esters gave the same product, 3-isopropylidene-2-coumaranone (III), m. 97.degree. (from C6H6-petr. ether, 1:3). Reduction of III with H over PtO2 followed by reaction with N2H4 gave o-HOC6H4(Me2CH)CHCONHNH2, m. 99-101.degree.. Excess Me2SO4 (2.26 g.) added to 1.57 g. III dissolved in 10 cc. 20% NaOH and 8 cc. MeOH, let stand overnight, heated 2 hrs. on the steam bath, the MeOH stripped off, and the residue taken up in 10 cc. H2O and pptd. with HCl gave 1.34 g. Me2C:C(CO2H)C6H4MeO-o (IV), m. 145.5.degree. (from C6H6-petr. ether). KMnO4 oxidation gave Me2CO, o-MeOC6H4COCO2H, and o-MeOC6H4CO2H.

IT **39581-62-9**, Crotonic acid, 2-(o-hydroxyphenyl)-3-methyl-, .gamma.-lactone
(prepn. of)

RN 39581-62-9 HCA

CN 2(3H)-Benzofuranone, 3-(1-methylethylidene)- (9CI) (CA INDEX NAME)



L50 ANSWER 161 OF 162 HCA COPYRIGHT 2003 ACS
49:53483 Original Reference No. 49:10260g-i,10261a Synthesis of some 3-benzylidenecoumaran-2-ones. Gripenberg, Jarl; Juselius, Borje (Inst. Technol., Helsingfors, Finland). Acta Chemica Scandinavica, 8, 734-7 (English) **1954**. CODEN: ACHSE7. ISSN: 0904-213X.

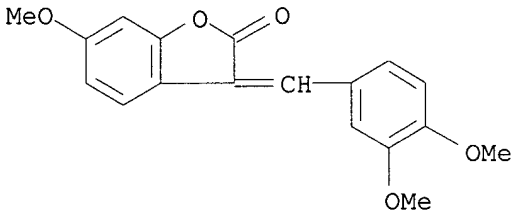
AB 3-Benzylidene- (I), 3-(4-methoxybenzylidene)- (II), 3-(3,4-dimethoxybenzylidene)- (III), and 3-(3,4,5-trimethozybenzylidene)-4,6-dimethoxycoumaran-2-one (IV), and 3-(3,4-dimethoxybenzylidene)-6-methoxycoumaran-2-one (V) were prepd. by condensation of a (2-hydroxyphenyl)acetic acid with the appropriate benzaldehyde. I to V m. 169.5-70.5.degree., 167.degree., 173-4.degree., 159-60.degree., and 183-4.degree., resp. 2,4,6-HO(MeO)2C6H2Ac (5 g.) heated 5 hrs. at 150-60.degree. with 2 g. S and 4.35 g. morpholine, the mixt. taken up in

CHCl3, the soln. washed with H2O and HCl, the CHCl3 removed in vacuo, the residue crystd. from EtOH, the thiomorpholide boiled with 20 cc. 30% KOH, and the alk. soln. dild. with H2O, extd. with Et2O, and acidified gave 0.8 g. 2,4,6-HO(MeO)2C6H2CH2CO2H (VI), which, taken up in Et2O, extd. with NaHCO3, pptd., the ppt. extd. with Et2O, and the Et2O evapd. in vacuo gave cryst. VI, m. 140-40.5.degree. (from Et2O-petr. ether); sublimation in vacuo gave 4,6-dimethoxycoumaran-2-one, m. 154.degree. (from Et2O). 2,4-HO(MeO)C6H3CH2CO2H (VII), m. 132-3.degree. (from Et2O-petr. ether), was similarly prepd. VI (1 g.), 0.55 g. BzH, 2 g. Ac2O, and 0.5 g. Et3N heated 6 hrs., 50 cc. H2O added, the mixt. boiled 15 min., and the product sepd., dried, taken up in Me2CO, and filtered through Al2O3 gave I; hydrolysis with 10% KOH and crystn. from C6H6 gave 2,4,6-HO(MeO)2C6H2C(CO2H):CHPh, m. 169.degree.. II was similarly prepd. (20 hrs. heating) from VI and anisaldehyde, III from VI and veratraldehyde (VIII), IV from VI and 3,4,5-(MeO)3C6H2CHO, and V from VII and VIII.

IT **6600-61-9**, Acrylic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4-methoxyphenyl)-, .gamma.-lactone **18087-47-3**, Acrylic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4,6-dimethoxyphenyl)-, .gamma.-lactone **64818-74-2**, Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(p-methoxyphenyl)-, .gamma.-lactone **102159-53-5**, Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)-, .gamma.-lactone **107153-09-3**, Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenyl-, .gamma.-lactone
(prepn. of)

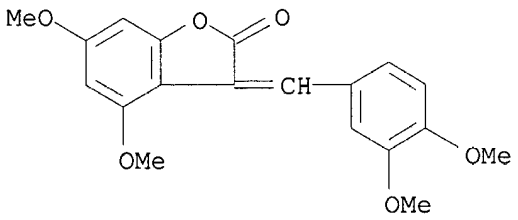
RN 6600-61-9 HCA

CN 2(3H)-Benzofuranone, 3-[(3,4-dimethoxyphenyl)methylene]-6-methoxy- (9CI) (CA INDEX NAME)



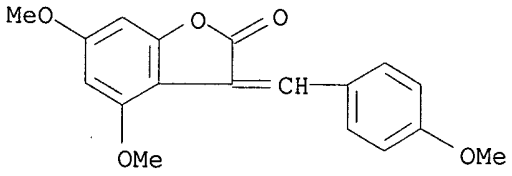
RN 18087-47-3 HCA

CN 2(3H)-Benzofuranone, 4,6-dimethoxy-3-veratrylidene- (8CI) (CA INDEX NAME)

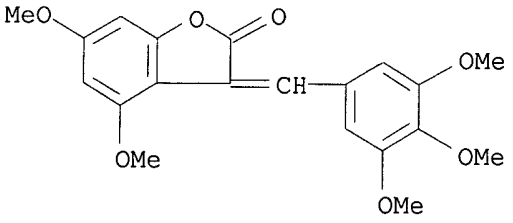


RN 64818-74-2 HCA

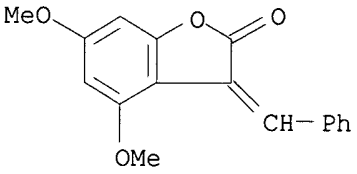
CN 2(3H)-Benzofuranone, 4,6-dimethoxy-3-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 102159-53-5 HCA
CN Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)-, .gamma.-lactone (6CI) (CA INDEX NAME)



RN 107153-09-3 HCA
CN Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenyl-, .gamma.-lactone (6CI) (CA INDEX NAME)



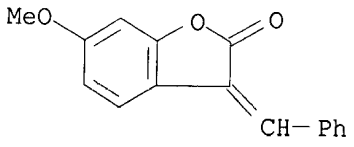
L50 ANSWER 162 OF 162 HCA COPYRIGHT 2003 ACS
41:32671 Original Reference No. 41:6555i,6556a-i The synthesis of oreoselone. I. Kumar, Satyendra; Ram, Labhu; Ray, Jnanendra Nath (Univ. Lahore, India). J. Indian Chem. Soc., 23, 365-70 (Unavailable) **1946**.
GI For diagram(s), see printed CA Issue.
AB An attempt is made to synthesize oreoselone (I). Friedel-Crafts reaction by gradual addn. of 14.8 cc. Me2CHCH2COCl in 12 cc. CS2 to 12.8 cc. m-C6H4(OMe)2 in 12.8 cc. CS2 and 10.5 g. AlCl3, refluxing the mixt., decompg. it with ice, and extg. with ether give 60% iso-Bu 2-hydroxy-4-methoxyphenyl ketone (II), b4 165.degree. (phenylhydrazone, fine needles, m. 85.degree.). Bromination of II gives an oil which when boiled with AcONa in EtOH gives a compd., m. 113.degree., which is not the expected coumaranone. Methylation of II by refluxing 26 g. in 90 cc. Me2CO and 21 cc. Me2SO4 with 50 g. K2CO3 gives a condensation product, Me2C[CH(CHMe2)COC6H3(OMe)2-2,4]2, m. 145-6.degree.. When into a mixt. of 5.8 g. BzHNCH2COCN, 4 g. m-C6H4(OH)2, and 7.7 g. ZnCl2 in 40 cc. dry ether, anhyd. HCl is passed until the oily layer is solidified, the mixt. kept 12 hrs. at 0.degree. and decompd., there is obtained 6.2 g. .alpha.-benzoyloxyresacetophenone, m. 200.degree., which does not condense with AcCH2CO2Et or malic acid (III). An attempt to alkylate 6-methoxycoumaranone (IV) with iso-PrI in the presence of EtONa or NH2Na failed. When 1 g. IV in 10 cc. Me2CO is refluxed 10 min. with 5 cc. 5% KOH, a condensation product, C21H20O6, of 2 mols. IV and 1 mol. Me2CO, m. 210.degree., is obtained. The analog, C22H22O6, from EtCOMe, m.

195.degree.. With aromatic aldehydes IV gives mono-mol. condensation products: benzylidene, m. 145.degree.; piperonylidene, m. 187.degree.; veratrylidene, m. 185.degree.; o-nitrobenzylidene, m. 199-200.degree.; 6-nitropiperonylidene, m. 250.degree.. When 1 g. 7-hydroxycoumarin in 0.6 cc. C5H5N is treated in the cold with Me2CHCH2COCl and the mixt. is warmed 5 min., 7-isovaleryloxycoumarin (V), m. 68.degree., is obtained. Fries rearrangement of 33 g. V with 7.5 g. AlCl3 45 min. at 70-5.degree., 45 min. at 120.degree., and 0.5 hr. at 135.degree. gives 7-hydroxy-8-isovalerylcoumarin (oxime m. 168.degree.; Ac deriv. m. 93.degree.), does not give a color reaction with FeCl3. 7-(.alpha.-Chloroisovaleryloxy)coumarin, m. 77.degree., does not undergo a Fries rearrangement. When 5 g. .beta.-resorcylic acid, 4.5 g. III, and 10 cc. concd. H2SO4 are kept overnight, heated 3-4 hrs., and poured onto ice, a mixt. of isomeric hydroxycoumarincarboxylic acids, m. 265-72.degree., is obtained and is sepd. by methylation with Me2SO4, whereby Me 7-methoxy-6-coumarincarboxylate (VI), m. 172.degree., is isolated by crystn. from EtOH. From the alc. mother liquors, Me 5-methoxy-6-coumarincarboxylate, m. 121-2.degree., is isolated and when demethylated with hot H2SO4 gives an acid, C10H6O5 (VII), m. 251-2.degree.. VII gives a deep violet color with FeCl3 and dissolves in dil. NaOH with a yellowish green fluorescence which fades quickly. Decarboxylation of VII gives 5-hydroxycoumarin, m. 225.degree.. Sapon. of 0.5 g. VI by heating with 7 cc. 10% NaOH gives 7-methoxy-6-coumarincarboxylic acid (VIII), m. 274.degree. (chloride (IX), prepd. with SOCl2, m. 190-1.degree.; Et ester m. 147-8.degree.; amide m. 297-8.degree.). Reaction of 2.4 g. IX with iso-PrNaC(CO2Et)2 in PhMe at 115-20.degree. 4-5 hrs. gives a condensation product (X) (Xa, R = CO2Et), m. 141-2.degree., which on hydrolysis gives VIII. IX and BrNaC(CO2Et)2 give a mixt. of compds. which are sepd. by extn. with petr. ether into crystals from dil. EtOH, m. 55.degree., and a compd. m. 140.degree.. Condensation of IX with BrNaC(CN)(CO2Et) gives a compd., C19H19O6N (Xa, R = CN), m. 156.degree., which when treated with H2SO4 gives a compd. m. 258-60.degree., not the expected coumaranone deriv. It is degraded with Ag-NH3 to VIII. When VIII is allowed to react with BuZnI in PhMe 2 hrs. at 0.degree. and 1.5 hrs. at 30.degree., the iso-Bu ester of VIII, m. 87-9.degree., is formed.

IT **4940-53-8**, Acrylic acid, 2-(2-hydroxy-4-methoxyphenyl)-3-phenyl-, .gamma.-lactone **6600-61-9**, Acrylic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4-methoxyphenyl)-, .gamma.-lactone
(prepn. of)

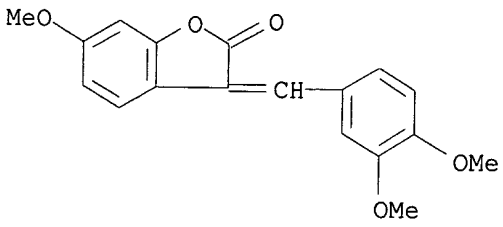
RN 4940-53-8 HCA

CN 2(3H)-Benzofuranone, 6-methoxy-3-(phenylmethylene)- (9CI) (CA INDEX NAME)



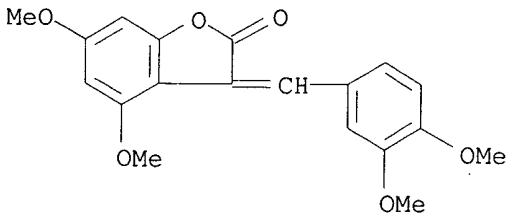
RN 6600-61-9 HCA

CN 2(3H)-Benzofuranone, 3-[(3,4-dimethoxyphenyl)methylene]-6-methoxy- (9CI) (CA INDEX NAME)

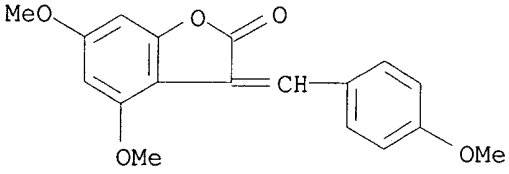

MeO
O
O
CH
OMe
OMe

2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(p-methoxyphenyl)-, .gamma.-lactone **102159-53-5**, Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)-, .gamma.-lactone **107153-09-3**, Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenyl-, .gamma.-lactone (prepn. of)

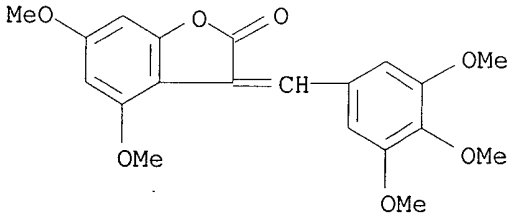
RN 18087-47-3 HCA
CN 2(3H)-Benzofuranone, 4,6-dimethoxy-3-veratrylidene- (8CI) (CA INDEX NAME)



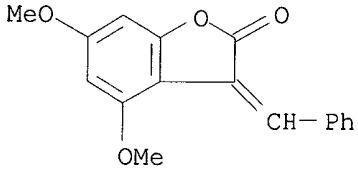
RN 64818-74-2 HCA
CN 2(3H)-Benzofuranone, 4,6-dimethoxy-3-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 102159-53-5 HCA
CN Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)-, .gamma.-lactone (6CI) (CA INDEX NAME)



RN 107153-09-3 HCA
CN Acrylic acid, 2-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenyl-, .gamma.-lactone (6CI) (CA INDEX NAME)



L50 ANSWER 155 OF 162 HCA COPYRIGHT 2003 ACS
51:43285 Original Reference No. 51:8063f-i,8064a-i,8065a-b Rearrangements of hydroxydiquinones. II. Rearrangement products of 2-hydroxy-4,4'-

ditoluquinone and of 2-hydroxy-4,4'-dimethoxydiquinone. Posternak, Th.; Huguenin, R.; Alcalay, W. (Univ. Lausanne, Switz.). Helv. Chim. Acta, 39, 1564-79 (French) **1956**.

GI For diagram(s), see printed CA Issue.

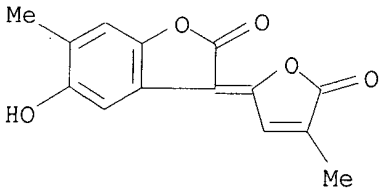
AB 2-Hydroxy-4,4'-ditoluquinone (I) (compd. VI of preceding part) (500 mg.) in 40 cc. hot MeOH treated with 20 cc. 10% H_2SO_4 and the mixt. refluxed 10 min. yielded 440 mg. 6,5-Me(RO)C6H2.O.CO.C:C.CH:CMe.CO.O (II, R = H) (IIa), m. 271-3.degree.. The rearrangement also took place in 70% AcOH at room temp., or in the same cold reagent starting with I, its acetate or its Me ether. IIa boiled 1-2 min. with 10 parts Ac_2O contg. 1 part anhyd. NaOAc yielded II (R = Ac), m. 214-15.degree.. II (R = $ClCH_2CO$) m. 249.degree.; II (R = o-ClC_5H_4CO) m. 233.degree.. IIa (1 g.) in 12 cc. hot N NaOH cooled, 3 cc. Me_2SO_4 and 16 cc. 2.4N NaOH added, the mixt. shaken 20 min., the reactions repeated 4 times, 16 cc. 2.4N NaOH added, and the product allowed to stand 4 hrs. and acidified to Congo red with concd. HCl yielded 0.74 g. II (R = Me) (III), m. 225-6.degree.. IIa (100 mg.) in 2 cc. AcOH heated to boiling, treated with 300 mg. Zn, filtered, and the filtrate poured into 10 parts cold water yielded 70 mg. butanolide analog (IV), m. 225-6.degree.. The butanolide analog (V) of III m. 174-5.degree.. IIa (1.2 g.) in 190 cc. hot AcOH cooled, treated with 4.65 cc. 6.07N CrO_3 in AcOH, allowed to stand 30 min., the products of 4 reactions united, poured into 3 vols. water, extd. with $CHCl_3$, the $CHCl_3$ evapd., the residue digested with 10 cc. EtOH, the insol. part taken up in 300 cc. $CHCl_3$, the soln. extd. 4 times with 100 cc. satd. Na-HCO_3, then with M Na_2CO_3, the Na_2CO_3 soln. extd. with HCl, then with $CHCl_3$, and the $CHCl_3$ evapd. yielded 112 mg. $(C_8H_6O_3)_n$, m. 313-14.degree. (cor.). The bicarbonate exts. washed with $CHCl_3$ and acidified yielded 1.58 g. OC.CH:CMe.CO.CH:CC(CO_2H): C.CH:CMe.CO.O (VI), m. 239-40.degree. (cor., decompn.). VI heated under N lost CO_2 and yielded a neutral product m. 254.degree.. VI titrated with iodine and the product decolorized with $Na_2S_2O_3$ and extd. with $CHCl_3$ yielded IIa. VI (46 mg.) treated at room temp. with 0.3 cc. 5% H_2SO_4 in Ac_2O and the product allowed to stand 4 hrs. yielded 45 mg. VII, m. 240.degree.. III (544 mg.) in 45 cc. hot dioxane cooled, treated drop by drop with 20 cc. 6% $KMnO_4$, filtered, the ppt. washed with aq. dioxane, the filtrates concd. in vacuo to 7-8 cc., the residue treated hot with 0.83 cc. 2.4N NaOH, these operations repeated 4 times, the alk. liquid concd. in vacuo to 1/3 vol., acidified to Congo red with 10N H_2SO_4, extd. 12 times with Et_2O, the Et_2O evapd., the residue in 10 cc. Me_2CO treated drop by drop (ice cooling) with 1 cc. 6% $KMnO_4$, filtered, the filtrate evapd. in vacuo, the residue in Et_2O shaken with $NaHCO_3$, and the ext. acidified and extd. with Et_2O yielded 4,2,5-Me(MeO)$2C_6H_2CO_2H$ (VIII), m. 124-4.5.degree.. VI hydrazinolyzed yielded the hydrazide (IX), m. 197-8.degree., of 4,2,5-Me(HO)$2C_6H_2CH_2CO_2H$ (IXa). The mother liquors yielded the dihydrazide (X) of mesaconic acid, m. 220.degree.. III with $N_2H_4.H_2O$ yielded the hydrazide (XI), m. 207-9.degree., of 4,2,5-Me(HO)-(MeO)$C_6H_3CH_2CO_2H$ (XII); the mother liquors yielded X, m. 221.degree. (decompn.). IV (100 mg.) with $N_2H_4.H_2O$ yielded 50 mg. IX, m. 196-8.degree.; the gummy residue from the mother liquors boiled 3 hrs. with 4 cc. 0.5N Ba$(OH)_2$ in MeOH, the Ba salt acidified exactly with H_2SO_4, the filtrate evapd., and the residue extd. with Et_2O yielded dl-methylsuccinic acid, m. 110-12.degree.. XI (100 g.) heated 30 min. in a water bath with 2 cc. 2N NaOH, cooled, acidified to Congo red with HCl, and extd. with Et_2O yielded 84 mg. XII, m. 121-3.degree.. 2,5-(MeO)$2C_6H_3Me$ (31.5 g.), 120 cc. concd. HCl, and 53 cc. HCHO (38%) treated 2 hrs. with a stream of dry HCl (the temp. held at 95-100.degree. during the 2nd hr.), and the mixt. cooled and extd. with Et_2O yielded 5-6 g. [4,3,6-Me(MeO)$2C_6H_2$]$2CH_2$ (XIII), m. 144-6.degree.. The Et_2O mother liquors yielded 17.3 g. 4,2,5-Me(MeO)$2C_6H_2CH_2Cl$ (XIV), b17 150-8.degree., m. 62-3.degree.. Molten XIV (13.2 g.) added to 40 g. NaCN, 65 cc. water, and 70 cc. EtOH, the mixt. refluxed 20 min., the EtOH distd., the residue

dild. with 1 vol. water, extd. with Et2O, and the ext. fractionated in vacuo yielded 1.30 g. 4,2,5-Me(MeO)2C6H2CH2CN (XV), m. 67-8.degree.; another fraction yielded 0.20 g. XV and a mixt. contg. 90% 4,2,5-EtO(MeO)2C6H3Me and 10% 4,2,5-Me(MeO)2C6H2CH2OH, which with dry HCl yielded XIV. XIV (1.15 g.) treated with NaCN and the residue sapond. with 6 cc. EtOH and 3.8 cc. water contg. 1.5 g. KOH yielded 700 mg. 4,2,5-Me(MeO)2C6H2CO2H (XVa), m. 131-2.degree., also obtained by methylation of 4,2,5-Me(MeO)C6H2CO2H (XVb). The hydrazide (1.78 g.) of XVa refluxed 7 hrs. with 50 parts 4N HCl, the HCl removed in vacuo, and the residue digested with 6 and 3 cc., resp., of water yielded IXa, m. 157.degree. (decompn.). IXa (220 mg.) distd. at 130-80.degree./0.1 mm. yielded 194 mg. 5-hydroxy-6-methyl-2-coumaranone (XVI), m. 163-4.degree., XVa (740 mg.) refluxed 1 hr. with 16 cc. 47% HBr, the HBr removed in vacuo, and the residue dried in vacuo over KOH yielded a mixt. of IXa and XVI which on distn. gave XVI, m. 161-3.degree.. XVb (50 mg.) heated 45 min. at 170-80.degree. (oil bath) yielded 30 mg. 5-methoxy-6-methyl-2-coumaranone (XVII), m. 104-6.degree.. XVI (78 mg.), 0.16 g. citraconic anhydride, and 0.02 cc. pyridine heated 4 min. at 155-60.degree. (the pyridine can be replaced by 5-6 mg. anhyd. NaOAc) and the cold mixt. dissolved in 2.5 cc. hot 2.3N NaOH and acidified with HCl yielded 70 mg. II, m. 272-3.degree.. XVI (69 mg.), 82 g. citraconic anhydride, and 7 mg. anhyd. NaOAc heated 10 min. at 155-60.degree. (oil bath), the cooled product treated with boiling water, and the residue recrystd. from AcOH yielded 44 mg. III, m. 226-7.degree.. 2,3,3',6,6'-Pentahydroxy-4,4'-dimethoxybiphenyl (3.1 g.) in 100 cc. boiling AcOH treated with 20 cc. water and 14.7 cc. 2.9N FeCl3 yielded 2.0 g. 6,5-MeO(R'O)C6H2.O.CO.C:C.CH:C(OMe).CO.O (XVIII, R' = H) (XVIIIa), m. 275-7.degree.; XVIII (R = Me) (XIX), m. 238-9.degree.; XVIII (R = Ac), m. 260-1.degree.. XVIIIa (333 mg.) in 1 cc. 99% N2H4.H2O allowed to stand overnight, the product evapd. to dryness in vacuo, and the residue treated with 0.8 cc. water yielded 95 mg. hydrazide, m. 198-200.degree. (decompn.), of 4,2,5-MeO(HO)2C6H2CH2CO2H; the aq. ext. contained CH2.CO.NH.N:CCONHNH2 (XX). XIX (200 mg.) treated 5 hrs. with 0.6 cc. N2H4.H2O yielded 55 mg. hydrazide, m. 177-8.degree., of 2,4,5-HO(MeO)2C6H4CH2CO2H; the mother liquors evapd. to dryness in vacuo, the residue treated with 0.5 cc. water and 0.5 cc. N AcOH yielded XX, m. 260.degree..

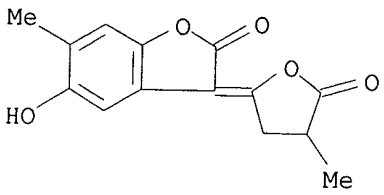
IT **80651-86-1**, Muconic acid, 2-(2,5-dihydroxy-p-tolyl)-3-hydroxy-5-methyl-, di-.gamma.-lactone **108487-90-7**, .alpha.-Hydromuconic acid, 2-(2,5-dihydroxy-p-tolyl)-3-hydroxy-5-methyl-, di-.gamma.-lactone **108900-07-8**, Muconic acid, 2-(2,5-dihydroxy-4-methoxyphenyl)-3-hydroxy-5-methoxy-, di-.gamma.-lactone **109342-75-8**, Muconic acid, 3-hydroxy-2-(2-hydroxy-5-methoxy-p-tolyl)-5-methyl-, di-.gamma.-lactone **109342-80-5**, Muconic acid, 3-hydroxy-2-(2-hydroxy-4,5-dimethoxyphenyl)-5-methoxy-, di-.gamma.-lactone **109442-63-9**, .alpha.-Hydromuconic acid, 3-hydroxy-2-(2-hydroxy-5-methoxy-p-tolyl)-5-methyl-, di-.gamma.-lactone
(prepn. of)

RN 80651-86-1 HCA

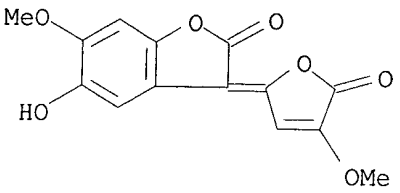
CN 2(3H)-Benzofuranone, 5-hydroxy-6-methyl-3-(4-methyl-5-oxo-2(5H)-furanylidene)- (9CI) (CA INDEX NAME)



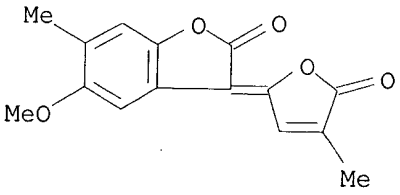
RN 108487-90-7 HCA
CN .alpha.-Hydromuconic acid, 2-(2,5-dihydroxy-p-tolyl)-3-hydroxy-5-methyl-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



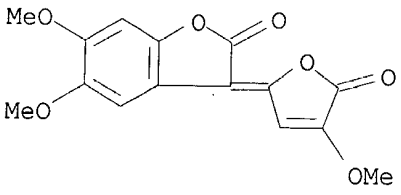
RN 108900-07-8 HCA
CN Muconic acid, 2-(2,5-dihydroxy-4-methoxyphenyl)-3-hydroxy-5-methoxy-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



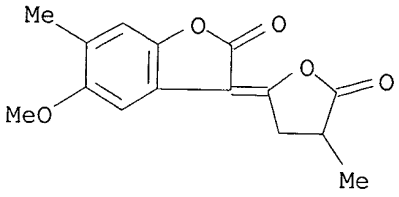
RN 109342-75-8 HCA
CN Muconic acid, 3-hydroxy-2-(2-hydroxy-5-methoxy-p-tolyl)-5-methyl-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



RN 109342-80-5 HCA
CN Muconic acid, 3-hydroxy-2-(2-hydroxy-4,5-dimethoxyphenyl)-5-methoxy-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



RN 109442-63-9 HCA
CN .alpha.-Hydromuconic acid, 3-hydroxy-2-(2-hydroxy-5-methoxy-p-tolyl)-5-methyl-, di-.gamma.-lactone (6CI) (CA INDEX NAME)



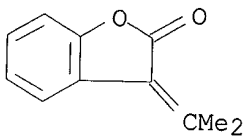
L50 ANSWER 160 OF 162 HCA COPYRIGHT 2003 ACS
50:1323 Original Reference No. 50:249b-d Claisen rearrangement of .gamma.-phenoxycrotonic acid esters. Canonica, Luigi; Fiecchi, Alberto (Univ. Milan). Atti accad. nazl. Lincei, Rend., Classe sci. fis., mat. e nat., 17, 385-90 (Unavailable) **1954**.

AB PhOCH2CH:CHCO2R (I) and PhOCH2CMe:CHCO2R (II) were studied under the conditions of the Claisen rearrangement. Besides a small portion which resinifies, I was recovered unaltered after 15 hrs. at 230.degree. or 270.degree. in an inert atm. This is an exception to the general reactivity of phenyl allyl ethers having a free ortho position (approx. 100 compds.) all of which rearrange at 180-220.degree. in 2-3 hrs. II (R = Me and Et) heated at 220.degree., however, rearrange, but the expected 2-(o-hydroxyphenyl)-3-methyl-3-butenoic esters were not obtained. Both esters gave the same product, 3-isopropylidene-2-coumaranone (III), m. 97.degree. (from C6H6-petr. ether, 1:3). Reduction of III with H over PtO2 followed by reaction with N2H4 gave o-HOC6H4(Me2CH)CHCONHNH2, m. 99-101.degree.. Excess Me2SO4 (2.26 g.) added to 1.57 g. III dissolved in 10 cc. 20% NaOH and 8 cc. MeOH, let stand overnight, heated 2 hrs. on the steam bath, the MeOH stripped off, and the residue taken up in 10 cc. H2O and pptd. with HCl gave 1.34 g. Me2C:C(CO2H)C6H4MeO-o (IV), m. 145.5.degree. (from C6H6-petr. ether). KMnO4 oxidation gave Me2CO, o-MeOC6H4COCO2H, and o-MeOC6H4CO2H.

IT **39581-62-9**, Crotonic acid, 2-(o-hydroxyphenyl)-3-methyl-, .gamma.-lactone
(prepn. of)

RN 39581-62-9 HCA

CN 2(3H)-Benzofuranone, 3-(1-methylethylidene)- (9CI) (CA INDEX NAME)



L50 ANSWER 161 OF 162 HCA COPYRIGHT 2003 ACS
49:53483 Original Reference No. 49:10260g-i,10261a Synthesis of some 3-benzylidenecoumaran-2-ones. Gripenberg, Jarl; Juselius, Borje (Inst. Technol., Helsingfors, Finland). Acta Chemica Scandinavica, 8, 734-7 (English) **1954**. CODEN: ACHSE7. ISSN: 0904-213X.

AB 3-Benzylidene- (I), 3-(4-methoxybenzylidene)- (II), 3-(3,4-dimethoxybenzylidene)- (III), and 3-(3,4,5-trimethozybenzylidene)-4,6-dimethoxycoumaran-2-one (IV), and 3-(3,4-dimethoxybenzylidene)-6-methoxycoumaran-2-one (V) were prepd. by condensation of a (2-hydroxyphenyl)acetic acid with the appropriate benzaldehyde. I to V m. 169.5-70.5.degree., 167.degree., 173-4.degree., 159-60.degree., and 183-4.degree., resp. 2,4,6-HO(MeO)2C6H2Ac (5 g.) heated 5 hrs. at 150-60.degree. with 2 g. S and 4.35 g. morpholine, the mixt. taken up in